Francesco Fontana

Molecular Manipulation in Augmented Reality

A User Experience Design applied research on new paradigms of interaction.

Master thesis

Aalto-yliopisto

Aalto University - School of Arts, Design and Architecture
Collaborative and Industrial Design (CoID) - 2018

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Dedicato ai miei amici,
a quelli presenti, assenti,
lontani, vicini,
a quelli persi e ,soprattutto,
a quelli ritrovati.

To all my friends,
to the ones present, absent,
distant, close,
to the ones lost and, most importantly,
to the ones found again.

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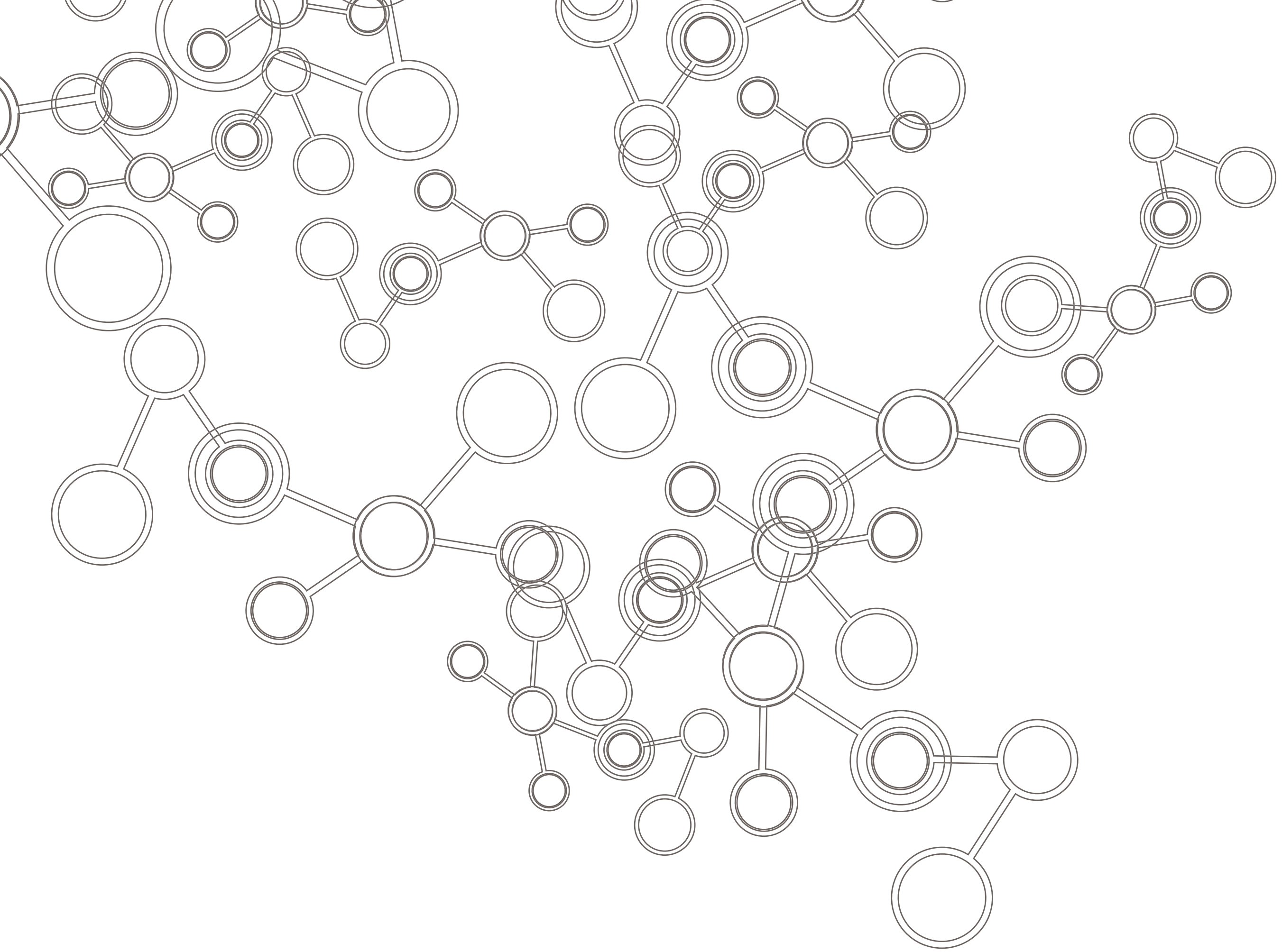
0. Abstract

This thesis presents the further developments of VR CHEM (2017), a molecular manipulation software in Virtual Reality. After evaluating a shift to Augmented Reality, changing consequently the name to AR CHEM, the project focused on this technology as it offers a competitive advantage for future development, especially considering the less invasive user experience and the incoming investments in the market.

The project is developed using HoloLens and Unity 3D as a platform, as these tools are considered the state of the art for AR technologies (2018).

The thesis presents a first iteration of new paradigms of interactions in AR: the 3D user interfaces and the Platform System. While the first explore the possibility of giving information to the user through 3D models used as UI/UX indications, the second strengthen the user's visual perception of depth in space, tying all the content to more tangible elements.

Keywords: *augmented reality, virtual reality, user experience, user paths, user interface, participatory design, Microsoft HoloLens.*



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1. Introduction

VR CHEM is a Virtual Reality (VR) molecular manipulation software that allows chemistry students and professionals to explore molecular relationships and reactions in a digital laboratory.

The tool offers a variety of interactions and it is based on existing mathematical models that ensure proper behaviour during the manipulation. The project is held by Aalto University School of Chemical Engineering, in collaboration with both Aalto University School of Arts, Design and Architecture, and Aalto University Department of Computer Science.

The research project started in April 2017 and explores the worlds of Virtual, Augmented and Mixed Reality. After a first prototype using VR, the researchers encountered many issues linked with this new means. Therefore, it was decided to pivot to Augmented Reality (AR), changing the name to AR CHEM. This second term will be used only in the latter part of the thesis, for clarity.

This Master Thesis continues the previous work in the shape of a practice-led applied research, a study "where the research leads primarily to the new understandings about the design practice itself (Candy, 2006)". Therefore, the research aims not only to design new features to tackle known issues, but also to envision the future the project's mixed reality UX for the next years. These objectives are pursued by designing a new user experience, evaluating Augmented Reality as a viable technological alternative for the future and ultimately defining efficient paradigms of interaction in AR.

Firstly, this introduction chapter aims to explain and present the development status of the project prior to this research, highlighting known issues and presenting an overview of the key feature implemented. Secondly, the chapter presents the research questions and defines in depth the aims of this applied research. Thirdly, the chapter explains the methodology used and offers an overview on the workflow.

1.1_ Previous Development

VR CHEM development started in April 2017 and by February 2018 it consisted in 2 versions of the same prototype: a traditional desktop software, and a virtual reality experience. Both versions share the core functionality, however, while the traditional desktop software uses mouse and keyboard as input methods, the VR version uses a Leap Motion controller and an HCT Vive Head Mounted Display. The researchers explored and compared the possibilities of these two versions, highlighting benefits and the limitations.

The aim of the prototype was to allow observation, creation and manipulation of molecules in a virtual environment, including also bond length, angles and atom saturation adjustments (Dhinakaran, 2017).
During the development of the prototype, a settings system (e.g. toggle rotation or toggle creation) was introduced allowing the usage of only one specific set of action at the time. However, it was soon clear to the researchers that a context sensitive UX would have performed better, as users often completed the correct actions using the wrong settings (Dhinakaran, 2017).

In the end of the research, the researchers organized a user test session to compare the performances of the Desktop Mouse and Keyboard interface with the one based on Leap Motion and Virtual Reality. The user test involved 11 people and consisted in 3 molecular manipulation tasks; each task required a sequence of precise actions in order to be completed (e.g. building an atoms fragment, creating bonds, rotate the molecule). The prototype had a built-in analysis tool to record the time used for each action and the number of undo performed for each task.

The results indicated that superiority of the mouse and keyboard interface mainly regarding speed, precision and feedback reliability (Dhinakaran, 2017). However, the user group agreed on the higher visual potential and clarity of the VR visualization compared to the traditional desktop software (Dhinakaran, 2017). The mouse and keyboard interface, as it was implemented, was also identified as harder to memorize by the users (Dhinakaran, 2017).

From the prototype design process and the user test, several other issues emerged, especially on the VR version. The Leap Motion hand gesture recognition is flawed and fails mostly when a natural wrist rotation is performed by the user (Dhinakaran, 2017). The prototype relied mainly on the pinching, grabbing and pointing gesture, as these were identified by the researchers as the most reliable ones (Dhinakaran, 2017). In addition, depth perception and precision issues emerged as users were missing the colliders of some objects when performing the creation action. Last, the VR user interface was fixed on the scene to the left of the user; the impossibility to move it and adjust it to the user preferences also brought to uncomfortable use cases, especially when involving left-handed users. While some of these problems could have been fixed with workarounds, Dhinakaran (2017) also believes that "mixed reality may solve several of these issues by offering the ability to use regular input devices while visualising virtual objects".

The main features of the prototype when this research project started was the following:

- *Select element*
- *Undo action*
- *Delete element*
- *Create atom or bond*
- *Create bonded atom*
- *Substitute Atom*
- *Cycle through bond, double bond, triple bond*
- *Stretch bond*
- *Rotate atoms using a bond as axis*
- *Rotation Snapping at 15°*
- *UI List of common atoms and a periodic table*
- *Automatic geometry optimizer according to the structure*

During this research, the aim was focused on improving the implementation of said features, designing UX AR paths for future developments, rather than extend the current feature set. In addition, at the beginning of this research project, it was decided to code refactoring the project, switching to a more recent version of Unity (from Unity 5.6.6 to Unity 2018.2) and restructuring functions and code interfaces for a smoother development. For this reason, several low priority features, already implemented in the first prototype, were left aside in the last prototype due to time constraints.

1.2_ Research Questions

Considered the 4 years length of the project and the previous developments, the aim during the 5 months long research project was to offer a guidance for envisioning and designing the future user experience of this software.

This research project was developed through 3 concatenative stages and, thus, 3 research questions:

- *What is the right technology for this project in the long term?*
- *What are the users' needs and wants?*
- *What UX in AR and VR can offer as a new paradigm of interaction?*

The first stage of the research focused on understanding whether the VR technology was the best choice to develop a molecular manipulation software, also considering market research and upcoming technological innovation. The second step was to understand, given the chosen technology, the hidden needs and wants of the user; instead of using competitor software features set, as done by previous research in this project, it was important also to confute the hypothesis with proper user research.

As a third and last step, knowing what the users will be looking for, the research focused on envisioning interactions to allow the best user experience, considering highly that AR and VR paradigms of interaction are still changing rapidly and there is little formal theory about it. Therefore, the concatenation of these three steps aimed to create a solid ground base for the future developments of the project.

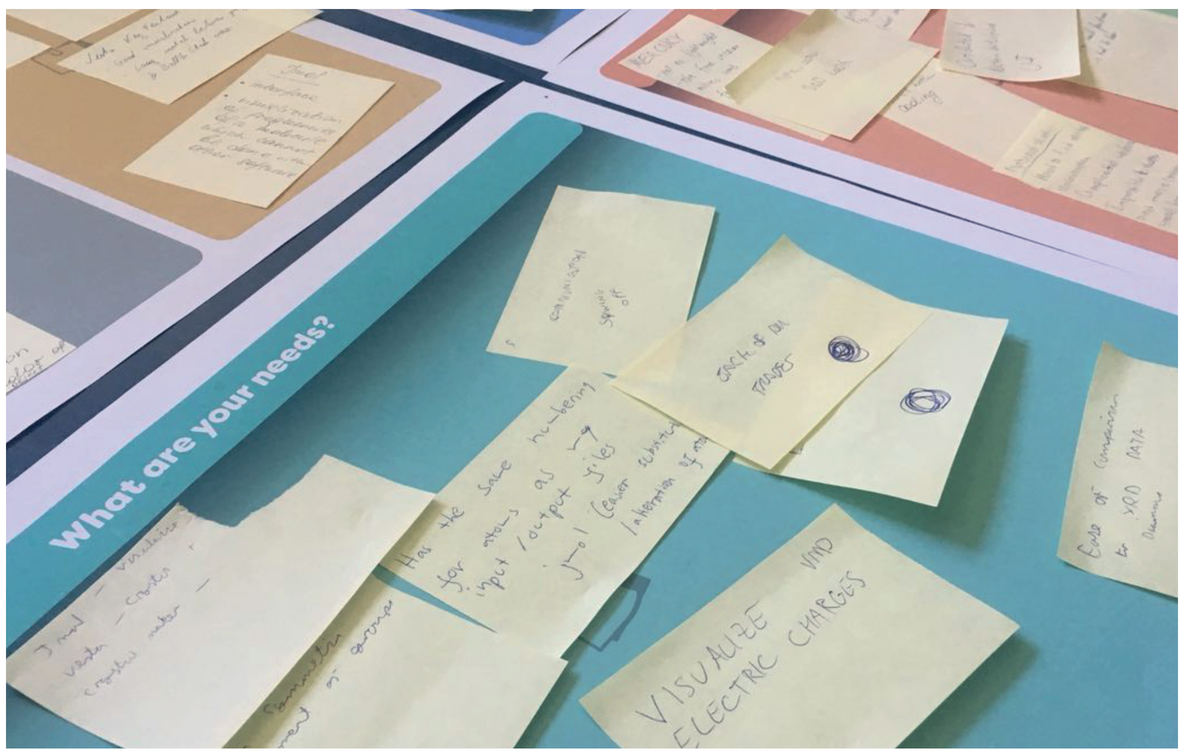


Figure 1.1 - Focus group results - Appendix (B)

1.3_ Methodology

To frame properly a design problem is the first and most important step to solve it (Muratovski, 2016). For this reason, a set of 5 methods was used to shape a methodology able to provide a solid understanding of the subject and empower an efficient design solution. This methodology includes:

- *Thematic Literature review*
- *Focus Groups*
- *Multi-platform exploration*
- *Fast prototyping*
- *User research*

1.3.1_ Thematic Literature Review

Thematic literature reviews mainly focuses on retrieving information about a specific phenomenon in his various aspects, providing an overall understanding across multiple fields (Muratovski, 2016).

In this research, the thematic review focuses on effective UX design practices in both traditional experiences and Augmented Reality ones, to provide a clear landscape on positive and negative UX practices and to fill the eventual knowledge gap during the development of this project.

For practical purposes, the literature is referenced throughout the whole research as intertwining the knowledge with the design process served better the needs of this project.

The sources used to conduct the review are:
- *https://aalto.finna.fi/*
- *https://scholar.google.fi/*
- *https://ieeexplore.ieee.org/*

Even though, officially, AR is already almost 20 years old, this technology is getting into our everyday life only recently (van Krevelen & Poelman, 2010). Every year AR becomes easier to access, from our phone to actual head mounted displays such as Microsoft HoloLens. With this change, the UX varies drastically from device to device and from year to year. Considering this dynamism, the review focuses mainly on articles and publications from the last 10 years when investigating AR practices. The review takes into consideration also UX guidelines and articles published by major companies such as Google.

1.3.2_ Focus Groups

Instead of focusing on structured or in-depth interviews, the research relies on focus groups. The main difference between these three method is that a focus group, while having a structure, still foster communication between the interviewees and creates a discussion around the topic (Muratovski, 2016). In this way, when investigating around users' needs and wants, it is faster to identify common pain points and recurrent topics to focus on. The collective feelings and expectation were the main focus and, therefore, it was chosen an interview method able to grasp them. During the first stage of the research, three focus group sessions were organized, with a total of 14 participants and collecting around 60 insights to work on. The focus group is explained in more detail in chapter 4 and in Appendix (B) and (C).

1.3.3_ Multi-platform exploration

During the research, the main difficulty was relying on very new and often clumsy technology. For this reason, to envision the future possibilities of AR UX, it was necessary to explore the issue through different platforms, triangulating different platforms and considering complementary benefits and flaws. Currently, considering industry reports, it is agreed that there is no reliable AR/VR device that is usable on a large-scale professional capacity (Forrester, 2018).

During the design process, used and explored three main platforms:

- *Microsoft HoloLens (AR)*
- *HCT Vive + Leap Motion see-through (AR)*
- *HCT Vive + Vive Controllers (VR)*

Our main platform was Microsoft HoloLens, as it offered the clearer immediate representation of the future of Augmented Reality. However, considered the many controls limitations, during the design process the team explored also the HCT Vive headset, used in see-through mode allowed by the Leap Motion, simulating an immersive Augmented Reality. The main limitations of this second tool were: a low quality black-and-white video stream, slight lag and the invasive nature of the headset. As a last, complementary tool, we used a plain HCT Vive using Virtual Reality. This tool was the most reliable and clear of all three. However, while this tool was good to test controls and manipulation, it was obviously the farthest simulation experience from AR.

1.3.4_ Fast Prototyping

Prototyping can offer several benefits, especially as it allows and facilitates early user involvement during software development (Brown, 2008). However, even before involving the user, prototypes paired with agile development are crucial, as it is not feasible to discover all the requirements of a project in advance when it comes to innovation (Boehm, 2000). In addition, as time constraints and technological change are common challenges when dealing with agile software development (Highsmith & Cockburn, 2001; Ramesh, Cao, & Baskerville, 2007), prototypes can be used to make requirements validation and refinement while keeping the process flexible (Ramesh et al., 2007). Moreover, it is argued that, when exploring novelty, an experimentation-driven approach can more likely generate good results (Ries, 2011), and it can facilitate the design process offering a concrete artefact as a base for discussion (Houde & Hill, 1997; Schrage, 2010), especially in multidisciplinary teams (Snyder, 2004). Prototypes can function also as documentation: nowadays many agile projects substitute prototypes to written design documents (Ramesh et al., 2007), smoothing considerably the readability of previous developments in long term projects. Lastly, prototyping can save actual development time if the final software is designed using the same or similar technology (Käpyaho & Kauppinen, 2015). For all these reasons, the team decided to implement fast prototyping as a main driver during the design process. As a consequence, during the research, small UX paths were designed and tested right away as much as possible, before involving systematic user testing.

1.3.5_ User research

The user research of this project can be thematically divided in two distinct part: UX research and Usability research. While the first is more centred on researching user experience paths, user's habits and previous user knowledge, the second is focused on usability, presenting precise features of a prototype and getting feedback to reiterate the design process. User experience and usability have many points in common as they both measure the quality of an interaction. However, while it can be argued that UX is the successor of traditional usability, it is simpler to consider these practices as two different ways to investigate the same problem: one looking at the big picture, and the other looking at the detail. This user research aims to formally use both methods in a complementary way. User experience, in fact, starts in a time frame that precedes and follow the concrete act of the interaction, while usability starts and ends with the actions of the user (Roto, 2009).

User experience, before the actual interaction, aims to understand the user's background and the general context in which the interaction will happen, considering the overall system (Roto, 2009). On the other hand, when usability focuses on the interaction, many approaches are possible. In fact, usability can be fragmented and used as a framework to analyse user feedback from different points of view (Hertzum, 2010). According to this theory, Hertzum (2010) defines six so-called "images" of usability, each one with a different focus on the interaction:

- *Universal Usability: focused on a system usable by everybody*
- *Situational usability: focused on the quality in use, which is particularly helpful in fast prototyping*
- *Perceived usability: focused on the user's subjective perception*
- *Hedonic usability: focused on what feedback generates a positive feeling in the user*
- *Organizational usability: focused on groups of people interacting in the same system at the same time*
- *Cultural usability: focused on the cultural perception towards specific features, very important while localizing software.*

On the other hand, regarding user experience, Marc Hassenzahl describes three qualities of the user experience, as cited by Lucero et al. (2014):

- *Stimulation: the ability to stimulate and enable personal growth*
- *Identification: the ability to address the need of expressing one's self through object one owns or mastered tools*
- *Evocation: the ability to evoke memories*

As evident from Hassenzahl classification of these hedonic qualities, UX encourages a way deeper understanding of user feelings and inner thoughts, without underestimating the concrete effect that these can have on the actual interaction (Lucero, Karapanos, Arrasvuori, & Korhonen, 2014). From these two schemes, it becomes evident how the focus of both practices can be complementary as they focus on the same problem but at different scales. In this research project, the UX research has been carried using focus groups in early development, and standalone UX tests during the advanced stages, such as the "perception and colour transparency" test, explained in Chapter 3. The user test relied on prototypes and traditional usability sessions. While testing with prototypes, there are some risks, especially in participatory design: during a user test, stakeholders might misinterpret the focus of the prototype version and may give feedback centered on features that are not meant to be tested during the session (Houde & Hill, 1997).

According to this, the main focus during the user test was to present only flows that were as complete and standalone as possible, so that the simulation could reflect the actual final product without distracting the user with known secondary flows of the prototype. This considered, giving multiple design alternatives of the same features could have generated a more valuable and realistic feedback during user tests (Tohidi, Buxton, Baecker, & Sellen, 2006). However, offering various alternatives for every feature is not always possible given the time constraints and the development difficulties; while prototyping, the team kept the principle in mind and applied it when possible.

Considered the time constraints, the user tests performed were restricted accordingly.

2. Augmented Reality or Virtual Reality?

2.1_ A market-oriented design research to choose the right direction

Even if in the past five years, Augmented Reality (AR) and Virtual Reality (VR) technologies have become increasingly more popular, these attempts are far from being novel. For example, the first attempt to produce an AR experience dates back to the 1960s, where Ivan Sutherland's team, between Harvard University and University of Utah, created the first AR display to show 3D elements (Van Krevelen, R., Poelman, R., 2010). Currently, 2018, the scenario is much more complex and the necessity to better define virtual and real spaces arises.

There are many definitions linked to VR and AR, according to the level of immersion and the kinds of interactions. It is also worth mentioning that these experiences can be achieved targeting different senses, other than sight (e.g. smell, hearing or touch); Last, the technology does not affect the definitions of the experience itself. "The ensemble between virtuality and reality is defined as Mixed Reality, a place where reality and the digital world meet at different degrees" (Van Krevelen, R., Poelman, R., 2010). As visualized in figure 1.0, these degrees of Mixed Reality are defined as follows:

- *Virtual Reality: virtual environment with virtual objects*
- *Augmented Virtuality: virtual environment with real objects*
- *Augmented reality: real environment with real and virtual objects*
- *Diminished reality: real environment with removed real objects in favour of overlaid virtual ones*

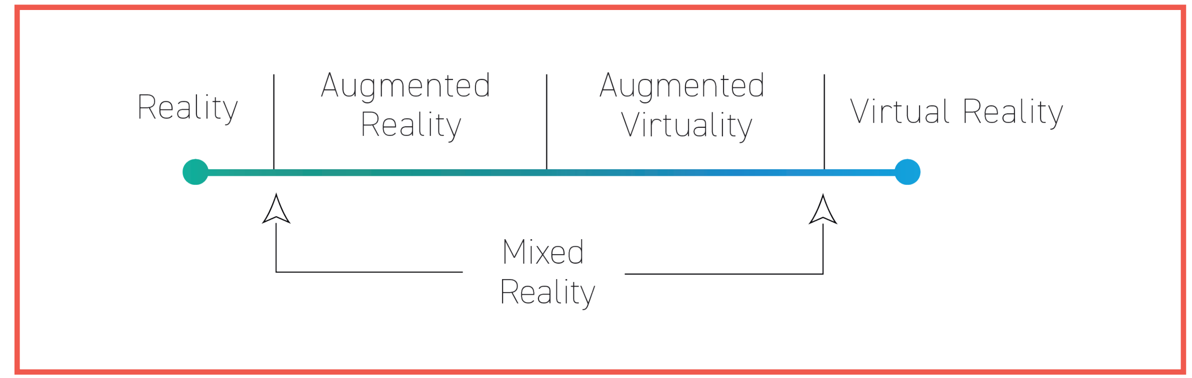


Figure 2.1 - Reality and Virtuality continuum (Milgram P., Kishino F., 1994)

Considering VR CHEM production needs, the research focuses on Virtual Reality and Augmented reality as the main paths for the user experience.

In the following chapters, the research evaluates the most notable advantages and disadvantages of both VR and AR, considering them according to VR CHEM's previous research findings.

The following chapters are highly based on confidential industry reports by Forrester.

The evaluation is based on the following framework:

- *Technology: general purpose*
- *Product analysis: quality of the interaction*
- *Forecasting: market direction*
- *Application to VR CHEM*

2.2_ Virtual Reality Evaluation

In the following chapter, Virtual Reality's state of the art is evaluated through a combination of literature review, industry reports and tech specialized newspaper articles.

2.2.1_ Technology: general purpose

VR is a powerful tool which projects the user into the digital world. The Guardian firmly affirms that, even though VR is risky to invest in, it is worth exploring due to the great empathy it can generate in the User (Forrester, 2018). Thus, VR has great potential in storytelling and narration, as the user can empathize with subjects and situations from the first-person point of view, as in real life.

In addition, Google expects that, in the near future, users will start capturing memories in VR, instead of taking 2D videos or pictures (Forrester, 2018). VR sends the user directly into a new environment, ready to see a world as it were the real one; the sensory experience is the strongest point of the headset. This becomes evident in the case of professional simulations like in medicine for surgery, or in a warfare context. Regarding the former, several programs exist to allow surgeons practicing complex operations with the help of a haptic pen (BBC, 2017); regarding the latter, the example comes from the Norwegian Army which allowed a soldier to drive a pilotless real tank thanks to a VR headset and a remote connection to the vehicle (Kamps, 2016). In these contexts, immersion in a new environment is the key to the experience, and could not be replicated with the same efficiency with AR.

2.2.2_ Product Analysis: Quality of the interaction

As Virtual Reality headsets come attached to a workstation, this can allow complex virtual environment creation impossible with the current AR technology. If this can be an obstacle for user's movements, it allows the developers to create much more complex scenarios using heavy computational power.

Taking a deeper look into how the technology works, the main aim of the VR headset results to be tricking the users' brain to simulate their body presence in a different environment. This phenomenon is known as telepresence (Van Krevelen, R., Poelman, R., 2010). To achieve this, the headset must create a stereoscopic vision, which consists of generating two images with a slightly different angle and feeding one for each eye. However, this is not enough to visualize the images correctly as the eyes are not able to focus on something that is too close. For this reason, between the display and the user's eyes, there are two focal lenses that allow a proper visualization.

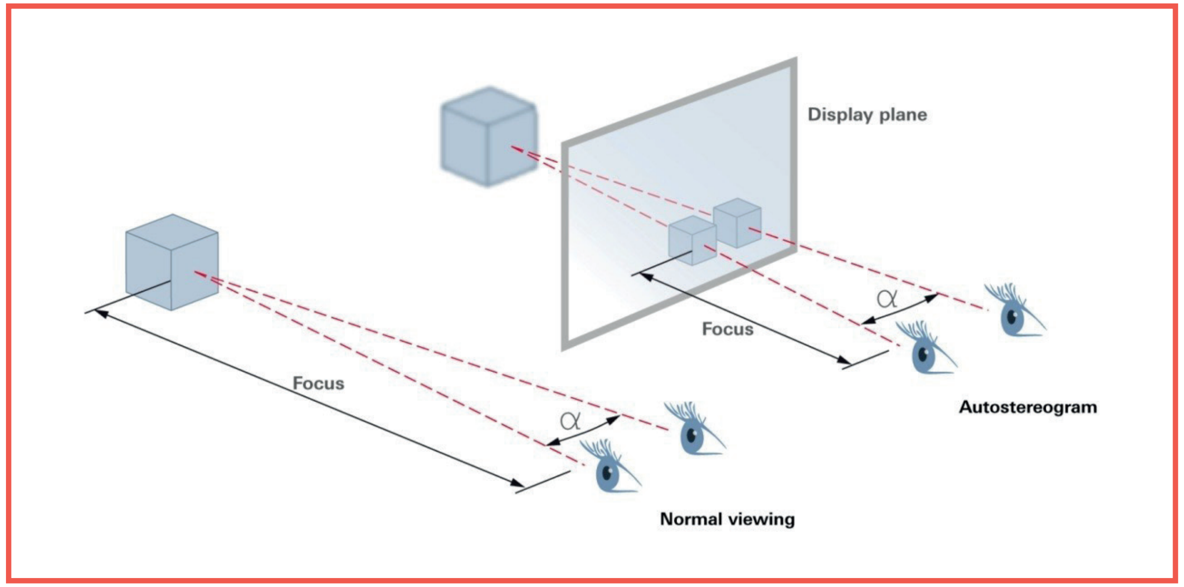


Figure 2.2 - Normal viewing and VR viewing (retrieved from https://www.quora.com/How-does-Virtual-Reality-VR-work)

The displayed scenes must always have a framerate of 60 fps or higher to result in a smooth experience. The last step to complete the visualization is motion tracking: if the user moves the head, the software should update the rendered scene accordingly and without any latency. This latency is known as Motion to Photon (MTP) and should be around 16.67ms in a 60fps scene. To detect the movement, the headsets use a combination of sensors like gyroscope and accelerometer, and, in the most advanced cases, they track also the whole user's position in space creating a much better feeling of immersion.

However, at the moment, Forrester experts considered the experience available still disembodied and unrealistic (Forrester, 2018). While the first refers to the difficulties in creating realistic avatars and animations that fit the user's body in the first-person view, the second refers to technical problems during the simulation. Such problems might include models colliding into each other, object disappearing or glitching elements controlled by the user when the tracking system is faulty. The experiences can also have a connection lag that causes motion sickness even with the slightest amount (Kamps, 2016) due to the current wired connection quality with the computer. At the current state, the most common user inputs (controllers and hand recognition) are still not versatile and comfortable enough to use to perform several tasks in the virtual environment (Forrester, 2018). For this reason, alternative controllers are being explored, among which haptic pens have represented a good solution but only for very specific types of interactions. In addition, the headsets themselves often presents affordance problems when the user quickly moves the head (Forrester, 2018); in fact, with the current ergonomics, most headset tends to slightly fall out of place due to the weight (0.5kg on average) and, if so, the user might visualize the content out of focus or unaligned with the sight. There are also side problems in the way current user experiences are built: many programs don't have proper controls explanation or headset setup instructions before the beginning of the use (Forrester, 2018). This may cause problems, especially during the focus setup, as the unfocused image itself can hardly help the user to setup the device. These side problems rise probably from the novelty of the tools and the consequent inexperience of the developers, as often happens with emerging technologies and tools. According to the above-listed problematics, it becomes evident that Forrester statement is solid: the technology is clearly not ready for mainstream diffusion among consumers and professionals.

2.2.3_ Forecasting: market direction

According to Digi-Capital, as cited in TechCrunch analysis, the AR/VR market will grow from the current 20 B to $108 B by 2021, with AR taking an up to $83 B and VR $25 B (Merel, 2017). While VR was outperforming AR back in 2016, the situation rapidly shifted in favour of AR and it is forecasted to grow way more rapidly than VR will do (Merel, 2017).

Despite the general market size growth is much slower for VR, most big players in the industry, such as Microsoft or Samsung, announced one or more VR headset alongside their main AR production. The reasons for a decrease in the investments in VR might be related to the current technologies as they allow more consumer-friendly experiences starting from a normal mobile phone, which is a way more familiar device than a headset. However, the advent of improved AI and 5G connection as mainstream could represent a hopeful solution to many of listed above problems as they are able to fix movement recognition without pad and create lag-less experiences.

However, these two technologies will not be mature enough before 2020 (Forrester, 2018). In addition, the headset requires an expensive high-end computer, roughly around a recommended 1500€ and it's itself around 600€, both on average [Hunt, 2018; Kamps, 2016; Oculus, 2018].

2.2.4_ Application to VR CHEM

Regarding the concrete application to the project, the perception of depth in VR was one of the key issues emerged by VR Chem previous research (Dhinakaran, 2017). When selecting, users had trouble selecting or pointing elements with precision. A lack of haptic feedback in VR was also partly responsible for this. However, overlaying buttons to real surfaces in AR could help the user having a better perception of depth.

A VR UI was also reported as a big challenge for the project, especially considering the great number of possibilities and data molecular manipulation requires. However, this problem relies less on the technology and more on how the user experience is built. Therefore, UI issues might emerge also in AR systems. In the chapter "New UI paradigms for AR and VR", the analysis goes deeper into the main issues of current interfaces with an analysis of the main available practices.

Leaving aside the technological issues, virtual reality represents a concrete advantage when it comes to simulating a whole environment for the user. However, VR CHEM does not need to simulate the surroundings around the user in order to accomplish its main task. According to the previous VR CHEM research, its main objective is to visualize a 3D interactable representation of one or more molecules to understand how further experiments or reactions can be designed. To do this, the focus of the experience is on the molecular model and on the user interface of the program; the surroundings are not involved into the process and offer only an emphatic working space for the user. However, as people are not used to virtual environments, its contribution is not a key for the experience and, therefore, it results less important than operating in the comfort of the real world thanks to an AR device.

The following paragraphs are going to analyse whether Augmented Reality represents a valid alternative to Virtual Reality now, and, most importantly, in the close future.

2.3_ Augmented Reality Evaluation

As for the previous section, in the following chapter Augmented Reality state of the art will be evaluated through a combination of literature review, industry reports and tech specialized newspaper articles.

2.3.1_ Technology: general purpose

As introduced previously, an Augmented Reality system can be defined as such when combines real and virtual objects in a real environment, aligns them with space and moves in all the three dimensions (Milgram P., Kishino F., 1994). AR empowers the user to add more layers of information to the real world, creating an enhanced version of it. The possibilities are endless but, in some fields, such as medicine or maintenance, AR really shows more clearly a disruptive potential (Azuma, 1997).

Regarding the former, it can be used to add additional information over a real patient during a difficult procedure, as presented by Fuchs et al. For laparoscopic surgery (Getting, 1993).

Regarding the latter, Honda and Volvo have manifested interest in using AR technologies to help technicians with vehicles history and repair procedure (Kaufmann, Schmalstieg, & Wagner, 2000).

AR can be also used collaboratively, which is a real game-changer. Different users, with headsets or other devices, can collaboratively interact with the same augmented environment, creating opportunities to implement professional work more easily and effectively.

At the moment, most collaborative experiences seem to be pioneered in the game development field.

2.3.2_ Product analysis: quality of the interaction

As stated in the previous paragraphs, these technologies can target also other senses. The first distinction in AR products is between aural displays and visual displays. The aural display can be obtained through different space dimensions: one in mono, two in stereo and three in surround mode.

However, real 3D aural displays are currently still not mainstream and are mostly paired with other AR or VR experiences. Aural displays also use haptic audio, a technology that allows to "feel more than hear" the sound, using heavier vibrations. Regarding Visual displays, there are mainly three categories of products:

- *Video see-through: a video is streamed on the display overlaying the environment (Azuma, 1997)*
- *Optical see-through: elements are visualized overlaying the environment (Azuma, 1997)*
- *Projective: a digital layer is physically projected over a real object (Azuma, 1997).*

In addition, each of this can be obtained through three kinds of means:

- *Head-attached: using a head-mounted display (HMD), with maximum immersion*
- *Hand-held: using a device such as a smartphone, watching through its screen*
- *Spatial: looking through a see-through fixed screen placed in the real environment*

Despite the researchers are working on all these methods but according to industry reports, handheld optical see-through experiences will lead the next generation in mixed reality (Forrester, 2018).

As all the new technologies, AR is far from being flawless. Currently, the main limitations can be summarized in:

- *Tracking and Calibration: despite the latest technologies, this remains a notable issue especially when it comes to complex hand gesture recognition. (R. van Krevelen & Poelman, 2010)*
- *Depth perception: without a wise use of the objects' shaders and materials, the user might encounter some difficulties in recognizing the proper depth of an object. (R. van Krevelen & Poelman, 2010)*
- *Overload and Over-reliance: overloading the user with complex UI is still an issue as there is little- documented know-how for AR user interfaces. (R. van Krevelen & Poelman, 2010)*
- *Battery life: current devices require frequent battery swaps as the hardware requires much power. (TechCrunch, 2018)*
- *App ecosystem: developers must keep investing in a technology that currently has not a solid user-base, however, this problem is common to all new technologies or platforms. (TechCrunch, 2018)*
- *Social acceptance: AR portable devices might still look odd if used in normal contexts, however, an improvement of the technology and the increasingly reduced size will tackle this issue in the future. (R. van Krevelen & Poelman, 2010)*

According to TechCrunch, a minor problem now is the lack of a true hero device that can lead the AR revolution. Smartphones can be considered the main platform AR platform at the moment, and probably in the future, according to market research (Forrester, 2018). Among these, very few devices (e.g. Google Tango) are designed to properly run satisfying AR experiences, and even those have battery and temperature issues. AR on smartphones is currently not ready but, according to the market direction, it will be more feasible by 2020 (Forrester, 2018). On the other hand, currently, there are available examples of standalone AR devices.

Microsoft HoloLens headset seems to be among the few to offer a complete all-around experience, including eye and hand tracking. However, these systems are by default still rudimentary and don't allow realistic high-precision manipulation without custom code.

2.3.3_ Forecasting: Market Direction

As anticipated in the previous chapters, investments in AR and VR are seeing a big turn of direction. The market is investing more and more in AR and this will foster a quicker growth in this sector, both considering the developers' community and the customer adoption. Forrester believes that the release of Apple ARKit with iOS 11 will tow more investors into AR technologies (Forrester, 2018).

Apple will quickly reach a wide audience making AR a mainstream technology (Forrester, 2018); therefore, users will be more and more familiar with these kinds of interactions.

In addition, Google announced ARCore: a new developer kit able to create modern AR simulations targeting not only the new mobiles but also the old ones (Forrester, 2018).

Facebook is now investing in AR opening Camera Effect Platform to the community, apparently shifting from a big previous investment in Oculus Rift (Forrester, 2018).

Other big companies have manifested interest in investing consistently in AR, following Google example; among these, we can find: Alibaba, Tencent, Samsung and Microsoft with its HoloLens visor. Even though at the moment, HoloLens represents one of the few unique examples of AR headset, most smartphone manufacturers will launch their own AR headsets by 2020 (Forrester, 2018).

In fact, according to Forrester forecast, only a small portion of US on-line population will have a VR headset by 2020, while AR will reach hundreds of millions worldwide by the same year (Forrester, 2018).

AR seems very promising and the direction of the market suggests a preference towards investing in AR technologies, first on mobile and then with proper hands-free headsets. Therefore, developing a 5+ years project such as VR CHEM might benefit a lot from using a technology that will see great growth in the close future, avoiding further pivoting and focusing on improving the program on a solid base.

2.3.4_ Application to VR CHEM

Implementing AR to the project can considerably improve the user experience. Despite VR allows us to display an interesting digital environment, VR CHEM does not need one itself, as it focuses on the visualization and manipulation of the objects. Along with that, removing the virtual environment and using the real space can help the professionals to feel more comfortable during the experience.

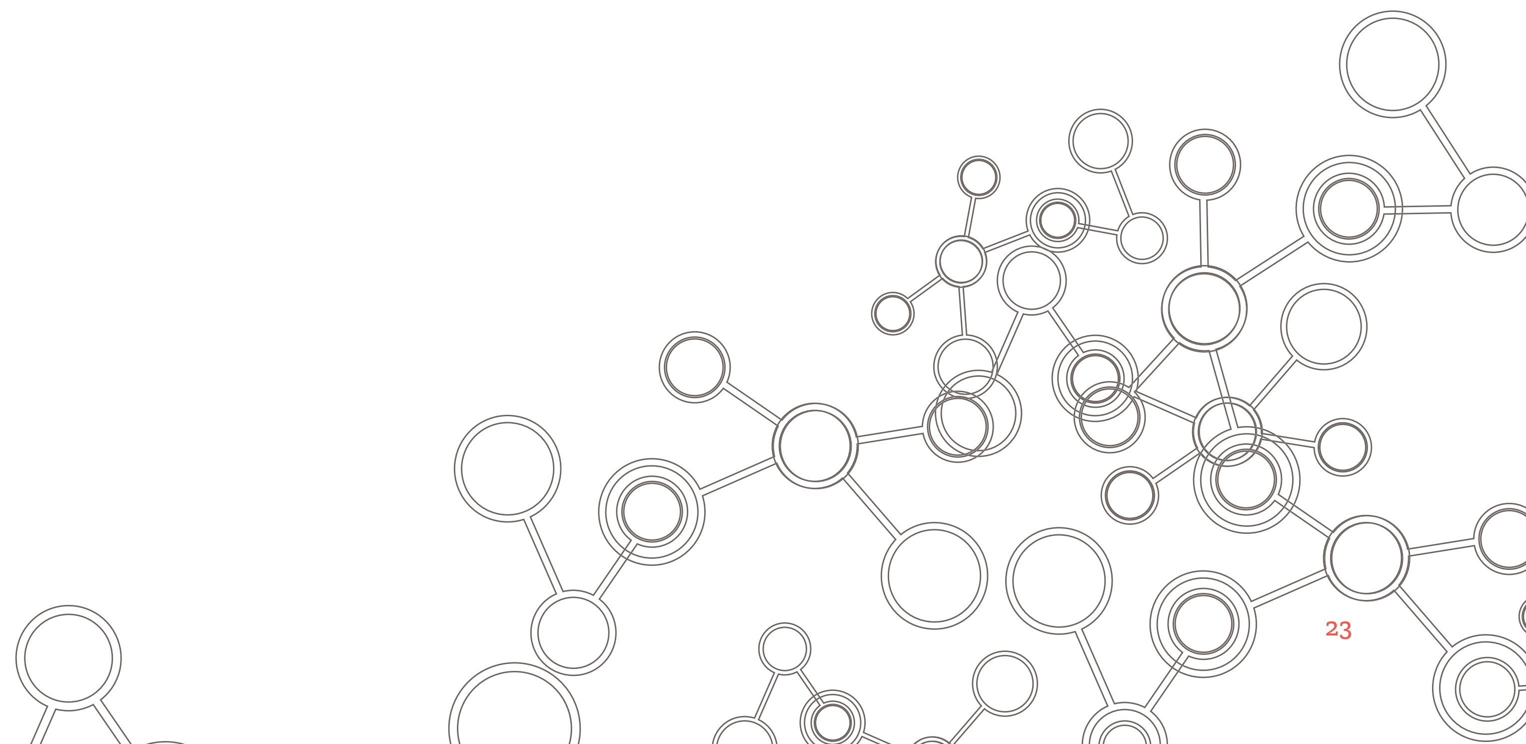
In addition, the setup of an AR headset such as HoloLens is much faster than the invasive VR counterpart. This considered, we must consider the possibility of AR collaborative environment, currently very hectic to achieve in VR. In future versions of the program, chemists could analyse and manipulate several molecules working in the same space on the same objects, allowing AR to become a true extension of their usual work routine.

Considering a practical perspective, according to a research conducted on 21 participants, recording 336 measurements, AR results to be quicker and more flexible than VR when it comes to 3D object manipulation (Krichenbauer, Yamamoto, Taketom, Sandor, & Kato, 2018). Despite the small amount of data, this research is worth mentioning as it studied object manipulation in ways that very much reflects the aims of VR CHEM.

The study recorded an 18% average time reduction for task completion compared to VR while using a mouse, and a 22% improvement while using a 3D control device (Krichenbauer, Yamamoto, Taketom, Sandor, & Kato, 2018).

Considering 8 hours a full day of work in VR, a chemist working with AR and a mouse will accomplish the same result in just 6h 34m, saving 1h and 26m.

Many of these improvements were attributed to a more comfortable view of user's own body and a better perception of space (Krichenbauer et al., 2018).



2.4_ Current paradigms for AR and VR

We can state that VR and AR provide different experiences with different methods, however, the paradigms of the interfaces have shared methodologies. Therefore, before analysing the individual technologies, this chapter will offer an overview of the common UI paradigms for AR and VR.

With new technologies come new interaction paradigms. WIMP user interface (windows, icons, menus, pointing) paradigm is not effective in an AR system (R. van Krevelen & Poelman, 2010), the same can be stated about VR. Even if AR and VR have some common necessities with traditional systems, such as selecting and text inputs, there is a big difference when it comes to keeping track of interactions and manipulations of real objects (R. van Krevelen & Poelman, 2010). The industry explored many ways to innovate the user interface (UI) paradigms.

The main new paradigms can be summarized in:

- *Tangible UI (TUI) + 3D pointing: a UI that uses real objects overlaid with virtual ones to simulate, for example, an HTC Vive controller as the equivalent of a usual mouse in a 3D space.*

- *Haptic UI + Gesture Recognition: a controller in the real world provides haptic feedback to the user, for example simulating forces like pressure, resistance, softness and hardness of a surface.*

- *Visual UI + Gesture Recognition: the user's hands are tracked visually without any additional controller, allowing gesture recognition thanks to image processing, for example with a Leap Motion.*

- *Gaze Tracking: users pupils' direction is tracked and recognized through cameras, allowing the user to point and select different elements of the digital UI.*

- *Aural UI + Speech Recognition: a UI that utilizes 3D sounds to provide information about the space, pairing it with speech recognition to allow user interaction.*

- *Hybrid UI: with complex AR programs a good practice is to implement multiple paradigms to provide more solid and effective user experiences, giving a variety of feedback and information to the user.*

2.5_ Conclusions

Considering the overview on the future investments, AR is growing at a much faster pace than VR and it will be the main player in the mixed reality market before 5 years. It seems convenient, for a long-term project such as VR Chem, to invest in such technology as it can result, on one side, in more funding or support, and, on the other, in better and more reliable tools.

Regarding the practical needs of VR Chem, it was presented how AR consists is a valid opportunity to improve the project, excluding an unnecessary virtual environment and making the users more comfortable, precise and efficient. Lastly, the importance of collaboration represents a real game changer when it comes to professional tools and, for VR Chem, it fits better the project's vision, allowing more chemist to collaboratively manipulate and study a complex molecule.

Even though neither AR and VR technologies are flawless, in order to design the general user experience, it is crucial to choose the technology that is going to fit better the users' and developers' needs, counting on support from the market and safely designing a long-term plan for the interaction. For this reason, Augmented Reality seems to be the best choice. As a consequence, the researchers decided to change the name of the project from VR CHEM to AR CHEM.

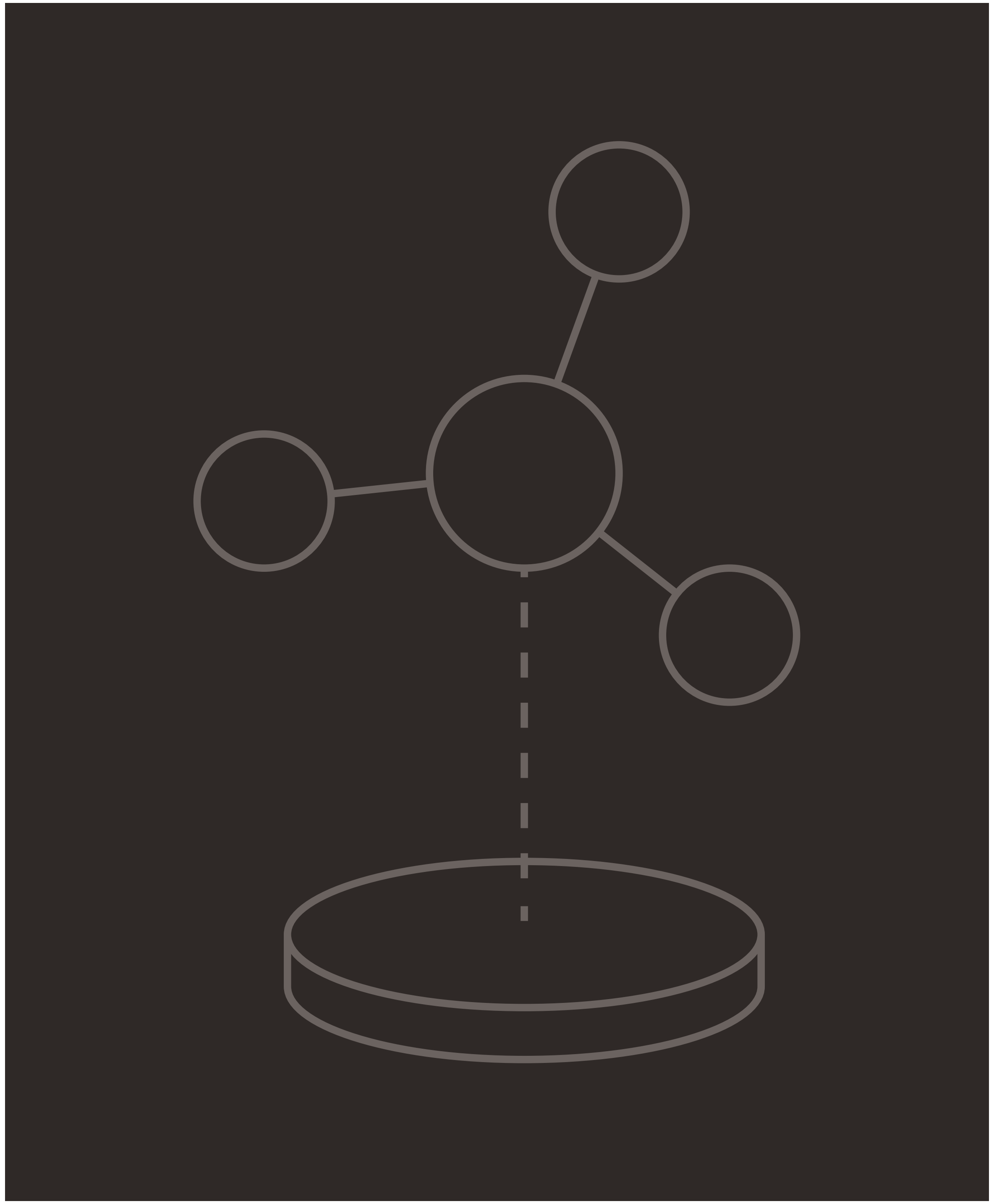


Figure 2.3 - Icon representing the Platform System, more information in chapter 4.

3. AR CHEM Development platform

Due to the shift to AR described in the previous chapter, the team decided to adopt HoloLens as the main platform to envision the future of UX interactions in Augmented Reality. This chapter presents an overview technical analysis of HoloLens and the tools used to prototype and test the software.

3.1_ HoloLens Analysis

In this paragraph, the research will present and reflect on HoloLens' most notable features (complete technical specifications list in Appendix (A)), analysing benefits and limitations. As the researchers used a multi-platform approach, this review will focus on the aspect most important for the specific needs of this method.

Benefits:

• *Non-invasive Standalone headset*
• *Reliable space mapping*
• *Reliable gesture recognition*
• *Holographic Quality*

Limitations:

• *Field of view*
• *Colours and Transparency*

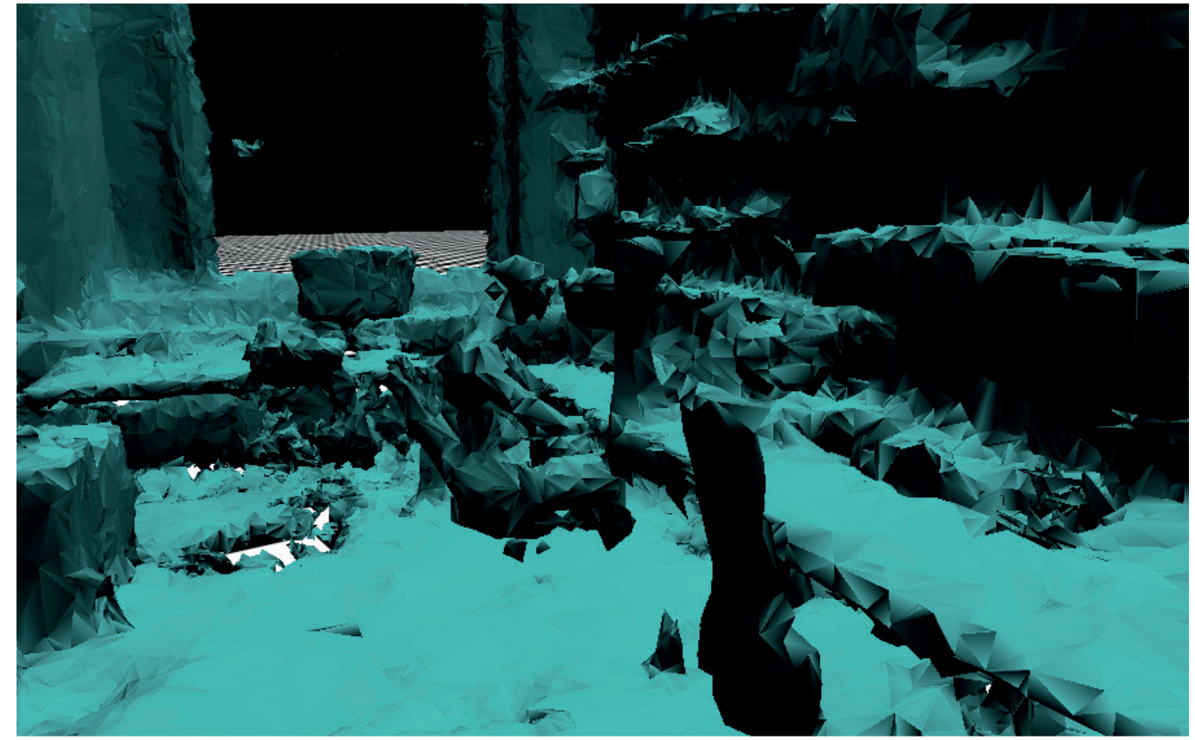


Figure 3.1 - HoloLens space mapping of the office. Kemistintie 1, 02150 Espoo , Finland.

3.1.1_ Benefits

HoloLens is a standalone headset (Microsoft, 2018), which means it does not require any external hardware to function properly. In addition, being an AR device, it does not aim for isolation, but it adds a layer of information to the existing world, creating a non-invasive experience for the user. This factor, as stated in the previous chapters, plays a key role in designing software meant to be used by chemistry professionals along with their usual workflow.

Regarding gesture recognition, HoloLens is far more accurate than the Leap Motion, used in a previous version of the prototype. Even though it offers a very restricted range of possible gestures, those allowed are reliable. This choice, compared to the Leap Motion, creates a better user experience overall, allowing the user to not generate false positives when clicking. During the development of the software the team organized a quick test to detect false positives using both devices, coming to the conclusion that HoloLens had a more reliable user input.

During the test, the user had to point and click on 250 spheres scattered around. The test was recorded using the built-in cameras of the HoloLens and the HTC Vive. Going through the footage, it emerged how the Leap Motion has many more blind or ambiguous spots than the HoloLens. For time and resources constraints, this test was only conducted between the researchers and does not represent a solid scientific evidence.

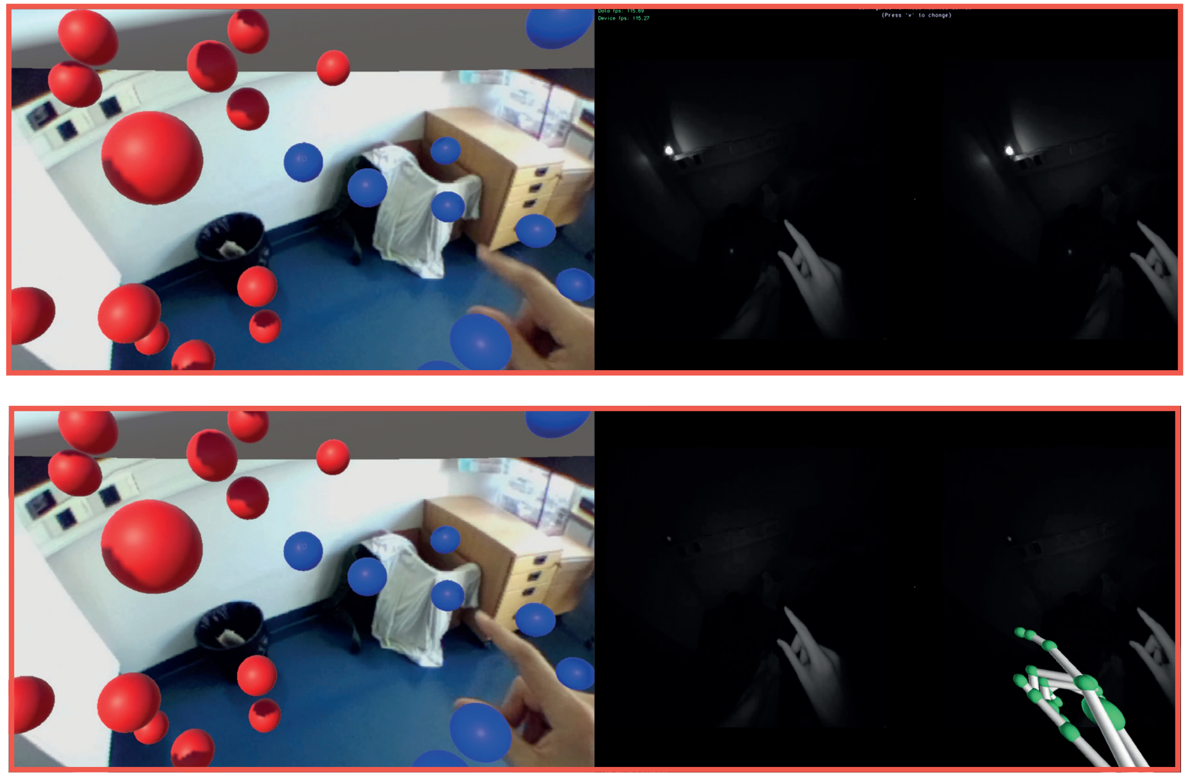


Figure 3.2, 3.3 - Footage recorded through the HTC Vive. A slightly different position affects the Leap Motion's ability to recognize the hand.

3.1.2_ Limitations

One of the main limitation of the current HoloLens model is the field of view. The users, in fact, are able to see the holograms only through a window in front of them, hence the immersion experience is not optimal with the current technological state.

However, Microsoft (2018) declared that the new announced model of HoloLens will have an improved version of the display, fixing the field of view problem. Therefore, for the purpose of this research, it was more important to focus on the visual perception of the high-quality holograms and the interaction with them, sacrificing the overall immersion experience.

Despite the very high holographic quality, HoloLens presents limitation in the colour spectrum available. In fact, HoloLens needs to render the colour black (Hex Code #000000) as transparent in order to function properly, hence the team had to find a way to simulate it; this need arose from common chemistry conventions which attributes the colour black to carbon atoms.

To solve this problem, Microsoft (2018) officially suggests to use dark colour instead (Microsoft, 2018), for example a dark green. However, while prototyping, the team felt the necessity to rely on more accurate data regarding colour perception, as dark colours were not always reliable in terms of opacity. For this reason, the team organized a colour perception user test. During the test, users were asked to sort colour tiles according to their opacity. Then, the users were asked to rank each tile from 1 to 10, trying to identify clear performance gaps in between the colour range.

The test was divided in three parts. The first was conducted first on grey scale tiles from pure black to pure white, the second was conducted on a RGB system with the whole colour spectrum, the third used the whole colour spectrum as a range but presented brighter colours (Test 01).. In this second part, every tile had a 15 units gamma variation on one channel at the time (Test 02)., while in the third, the variation was of 15 units on two channels at the time, producing brighter colours (Test 03).

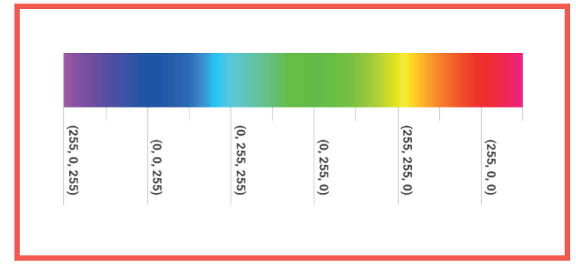


Figure 3.4 - Color range with maximum saturation

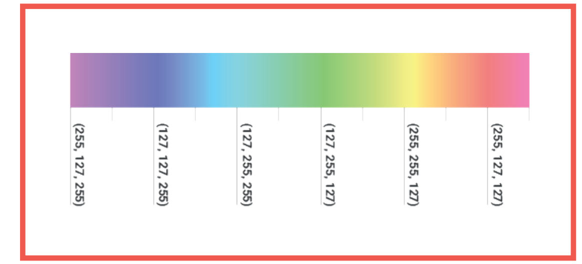


Figure 3.5 - Color range with lower saturation

Through this sequence, the test aimed not only to provide a clearer idea of the perceived colour opacity, but also to get insights on the most reliable colours in terms of usability.

The following diagrams show the result of the perception test, conducted on 7 people. Given the low number of participants, the test cannot offer strong scientific evidence, however, the consistency of the results allowed to identify some patterns, especially considering the standard deviation, identified by the grey vertical bars.

During this test, the team expected to see a better performance of the brighter gammas, but it was unclear how to define a safe range of use.

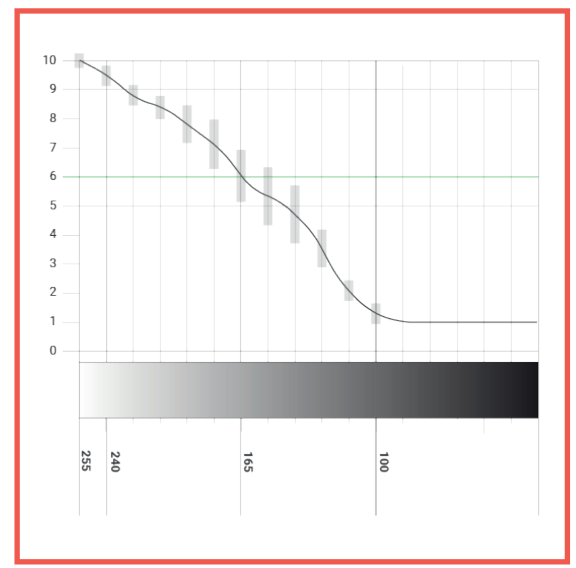


Figure 3.6 - Test 01: Grey scale visibility test with standard deviation

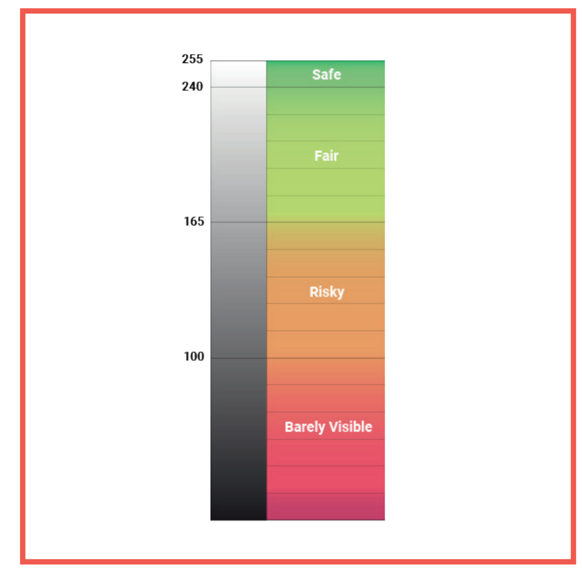


Figure 3.7 - Recommended gray scale values on HoloLens

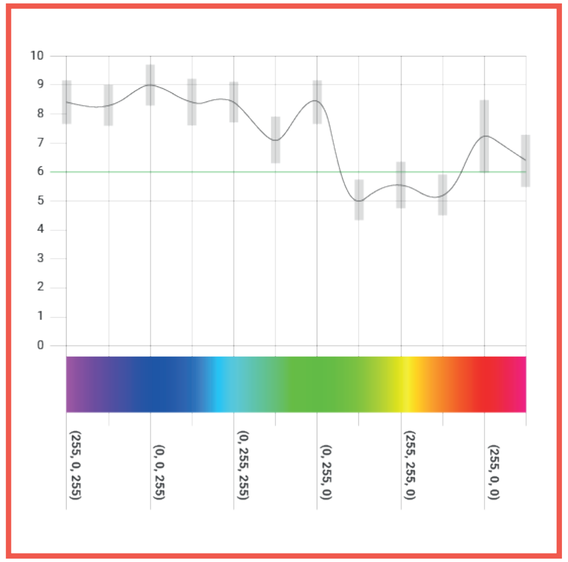


Figure 3.8 - Test 02: saturated colors visibility test with standard deviation

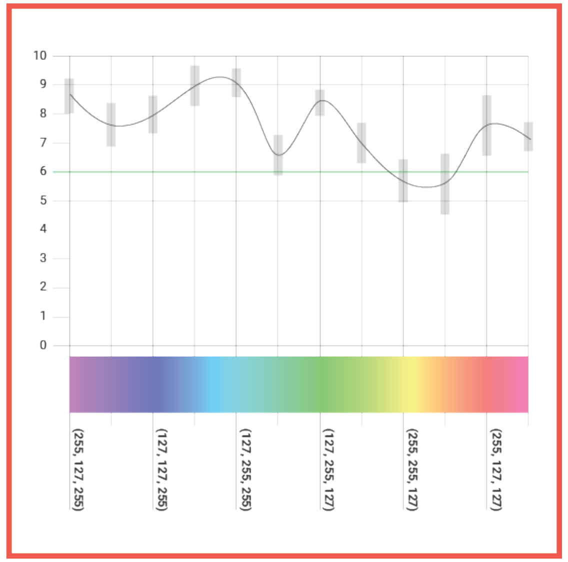


Figure 3.9 - Test 03: lower saturation colors visibility test with standard deviation

First of all, the average standard deviation in test 03 is lower comparing to test 02, meaning that those color tiles were easier to distinguish and rate. In desaturated colors, the light color is closer to white, hence it is more visible from the headset than darker colors.

In addition, the results presented an unexpected outcome: the color range from yellow to red demonstrated the lowest performance, even with their brighter versions.

Therefore, the team decided to avoid such colors during the implementation. Considering the stated conclusion, we can affirm that the study managed to partly clarify the overall user color perception on HoloLens.

Further studies could verify the results with a high number of testers, including also other gradations of color and testing against different backgrounds.

Data available at https://goo.gl/qDn6h9

3.2_ Unity Implementation

Unity 3D offers a built-in integration with HoloLens; however, the workflow is far from being flawless, which caused several workarounds and the impossibility to have a stable software build by the end of this project.

The prototype is available to be experienced through the Holographic interface provided by Unity: an add-on that connects the headset to the computer as Unity is running.

The impossibility to produce a software build came from the development choice of using the new Light Weight rendering pipeline: the new Unity standard for Augmented Reality. As the project will have a lifespan of at least 5 years, the team agreed on switching to the newest technology available to develop the features, waiting for Unity to release updates and fixes specifically related to HoloLens.

Developing the software on older standards would have allowed the creation of a software build, bringing, however, performance issues and unnecessary difficulties with outdated tools, such as the shader scripting. Considering the research and the aim of envisioning possible user experiences in AR, the outcome of the research was not heavily influenced by this workflow.

Figure 3.10 - The office setup viewed through Microsoft HoloLens

4. AR CHEM designing the User Experience

In this chapter, the thesis presents in detail the initial user research (workshops and focus group), then it explains the design of the User Experience paths, starting from the concept of 3D Icons and then presenting the Platform System.

AR Chem offers a variety of functionality but, considered the high amount of flexibility required by the users, the software must offer versatile flows able to concatenate different procedures, reiterate quick actions, recognize contextual situations and offer a vast plethora of options for the interaction.

After introducing the concept of 3D UI, this chapter presents the Platform System emerged as a result from the design process and the user flows of the main functionality for each platform.

While the first explain the concept behind the execution, the second one explores, from a practical point of view, the actual information the user goes through, step by step.

4.1_ Focus Groups

This paragraph introduces first the so-called double diamond design process in order to explain the concept behind the initial user research. Afterwards, the focus groups are presented in details, as anticipated in the previous chapters.

The design process was heavily based on the double diamond design process. The double diamond is a practice theorized by the Design Council (2015), which consists in four key steps: discover, define, develop, deliver. The peculiarity of the double diamond is the diverging and converging nature of the process (Design Council, 2015).

The designers start from an initial problem and, before developing a solution, they focus on exploring the problematic in its ecosystem (Discover) (Design Council, 2015). In a second phase of the first diamond, the research converges, clustering research finding and defining a clear, concise and efficient design brief (Define) (Design Council, 2015).

A design brief is "a written description of what a new project or product should do, what is needed to produce it, how long it will take" (Cambridge Dictionary, 2018). At this point, the designers have a clear idea of the problem, its surroundings and all the elements involved in its complex ecosystem; it is possible, then, to start developing solution (Design Council, 2015).

In this part of the process, the team explores several possible ways to solve the problem, in another diverging phase (Develop). As a last step, all the solutions are clustered and the best one is picked to be finalized and polished (Deliver). The steps inside the same diamond can be iterative, going from one phase to the other and vice versa (Design Council, 2015).

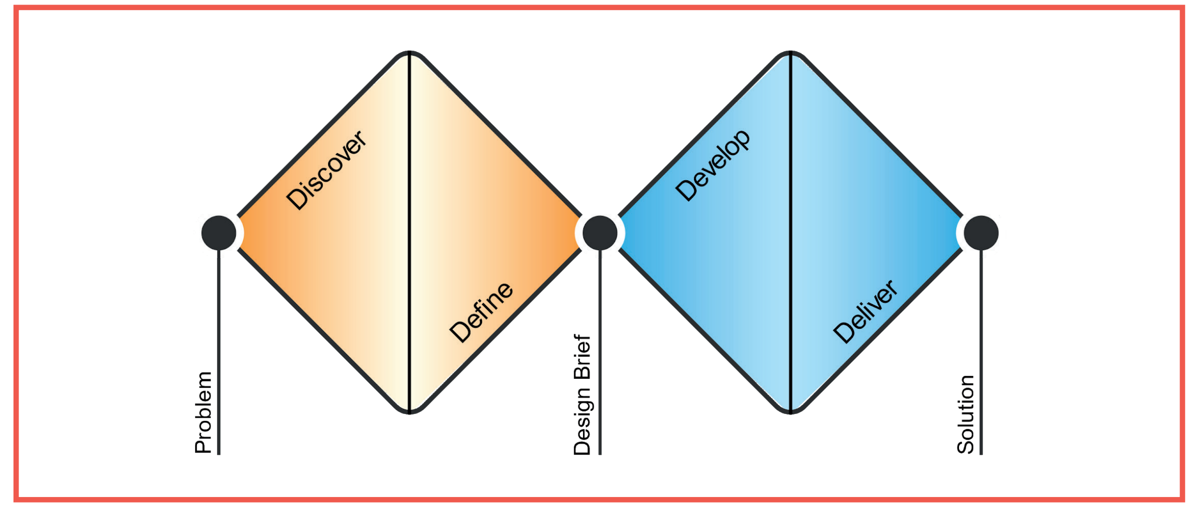


Figure 4.1 - Graphic representation of the Double Diamond Structure (Design Council, 2015)

Based on this process, the first two steps consisted in exploring the problems the users had, their background and their previous knowledge in similar softwares, while, at the same time, researching literature and formal knowledge in the field. For these reasons, three workshops were organized in the form of focus groups. The aim was to obtain key insights to start developing the software in a clearer direction, ensuring that users' needs and wants were taken into consideration.

Each workshop had a defined agenda, sent in advance via email to the participants. In addition, an online profiling survey was sent to gather data about the level of experience the users had in the field of chemistry; however, all participants were chosen among students and professionals in the field of chemical engineering. During the workshop, the project was presented and the aims of the sessions were explained. As a first step, the participants were asked to write down on a labeled board the main needs related to their work in relation of the software they were used to adopt.

Afterwards, the participants were asked to write down the name of the programs, presenting the key features. All the answers were marked on a labeled board. The same procedure was used to mark down flows and possible improvements to the marked existing programs. As a last part of the workshop, the features of the project were presented, at the state of the first prototype (2017).

While the first steps were key to better understand the users' background, the last one was the most valuable part of the workshop from a development perspective. Going through the feature list, all the participants gave a key contribution in suggesting main features that were missing, or simple adjustments to existing ones. By the end of the process, three workshop sessions were organized, with a total of 14 participants and over 60 clustered insights through affinity diagrams. The results of the workshops and the literature research carried in parallel were key to define the next steps. In the next chapter, the thesis presents the 3D User interface concept and the platform system.

Figure 4.2 - Focus groups participants profiling

4.2_ 2D and 3D User Interface

As carefully explained by Soete and Perez (1988), every new technology has a high initial cost for a company to research and implement best practices. This curve is decrescent and starts from a potentially infinite amount and arrives to a stable lower amount after a certain time (Soete & Perez, 1988).

This cost can vary according to the technology and to the approach the company is taking (Soete & Perez, 1988). For example, the company should heavily invest and research to obtain a comprehensive understanding of the new technology (Soete & Perez, 1988).

During this process, many companies feel tempted to implement old knowledge into the new field (Soete & Perez, 1988). This is defined by Soete and Perez as past "wrong experience" and it is advised to start fresh and avoid using it. This is visible in recent technology more than ever, for example, in the field of social computing. Social Computing explores the social environments and the data produced by users in the digital environment (Mabillot, 2007; O'Reilly, 2007; Pascu, Osimo, Turlea, Ulbrich, & Burgelman, 2007).

This practice was active before the advent of smartphones and mobile social computing, however, in the first years, companies did not realized the true potential of social computing applied to mobile, as they were focusing on their own old knowledge. For this reason, mobile social computing was considered only a "complementary means of access to social computing applications while on the move" (Feijòo, Pascu, Misuraca, & Lusoli, 2009).

Looking at the current scene, it is easy to observe that a big part of the modern AR and VR user interfaces do not apply this lesson. Therefore, there is room for big improvements and this thesis aims to be the first microscopic step towards it.

To start it was necessary to look back at previous innovations. As an inspiration, stepping few years back in time, one current stands out in the field of UX design: Google Material design on mobile platforms.

This approach was a great revolution and has still many valuable lessons that could be applied to design new UX paths in AR, not from a practical point of view, but from the perspective of the design process followed and the key concept referenced. In the following paragraph the thesis showcases the key points of this movement, and why was crucial as an inspiration for the design of the platform system and the 3D UI.

4.2.1_ From Google Material Design to 3D UI

Google Material Design is based on the concept of bringing the real qualities of the 3D space we live in, inside the mobile experience (Google, 2018b). Google aimed to bring the physical quality of paper interaction, into the digital world. Every design choice reflects this vision. The movements of the suggested guidelines for the swipe emulate the act of browsing a book or a newspaper (Google, 2015).

In addition, introducing paper-like qualities brought to an innovation in the field of UI hierarchy. In Material Design, every element has a Z depth level, and project shadows accordingly; this is key to understand hierarchical relationship between the elements, for example what is the header and what elements form the content of a particular screen (Tech Republic, 2018). According to Google's designers' interviews, this concept arose from the pure study of simple paper sheets and their behavior (Google, 2015).

Excluding the digital world as a very first step, was a solid design process that inspired the next steps of this research. In addition, Google dared to bring the 3D space into the 2D world, mixing the intuitiveness of the real world with a mobile user experience (Google, 2018a).

This inspired a consideration during the research: commonly, AR UI were bringing the 2D world into the 3D environment. This sounds once again an old experience of a paradigm used in a new technology and identifiable as an old "wrong experience" (Feijòo et al., 2009).

According to this consideration, it is arguable that the Augmented Reality can benefit from the presence of 3D UI elements in the real space, avoiding a forced 2D paradigm where not needed.

Starting from these concepts, a first iteration of a 3D user interface was designed. By this, it is not intended 2D UI in a 3D space, but real 3D models used as user interface elements. 3D models used as UI elements offer a clearer indication of their position in space in relation to the user; in fact, it is much harder to understand rotation and scale of a plane, being an object without shadows or occlusive parts.

Naturally, a selection of 2D UI elements was still used for practical reasons, such as text messages, loading icons and the mouse cursor. These elements did not need a presence in the 3D space for two reasons: they were mostly static, and they were not interactable.

If mobile UX learned a lot from web design, the 3D UI can learn a lot from traditional product design, where the shape of the object and its affordance was key to deliver the best experience to the customer. For this reason, the researchers put a specific attention in developing the right shapes to communicate the respective functions. From the first iteration of the 3D UI, the platform system was born as a consequence.

4.3_ Platform system

Reviewing UX best practices and being inspired by Google's Material Design in particular, an untapped potential arose. As presented in the previous chapter, implementing actual 3D interfaces can innovate the AR common UI approach. In this chapter, the thesis presents the Platform System. The Platform System is a first iteration produced as a result of the background research presented in the previous chapters.

As Augmented Reality wants to add a layer of information to reality, the usage of actual 3D models instead of floating 2D UI could be a step ahead in AR User Experience paradigms. The platform System suggests a simple idea: every element in the augmented world, called Content, lies on a 3D model, called Platform, and it is linked to it through several features.

Using a platform upon which instantiating content satisfies two main concerns that arose from the research: the problematic perception of the surrounding space, and the imprecise interaction with the augmented world. These two problems are intertwined with each other, and solving one affects positively parts of the other, and vice versa. For example, as the platforms interact with a real surface by laying on it, the user can perceive it as more concrete and connected to the real environment, guessing the distance more accurately and consequently interacting more precisely.
This results in easier manipulation and precision during the whole experience. On the contrary, floating elements are harder to collocate in space, especially when it comes to depth, as stated in the previous chapters. With the platform System, the user can have a clearer understanding of the AR work space and can manipulate, move and interact with the elements having a more cohesive and reliable perception of the space. In addition, connecting the platforms with their respective Content solves several problems encountered by the researchers in the previous Virtual Reality Prototype, first of which the impossibility to control scale or movement of the whole structure. With the platform system, to scale the Content, the user must scale through the relative platform, bringing the interaction from several elements, such us all the molecules, to just one that is always available and easy to reach.

The Platform System consists in a group of four Platforms, one for each cluster of features: Main, Tool, System and Utility. Each platform has a dedicated behavior and it is distinguished by the others in clear visual cues using the previously discussed 3D Icons. The system is designed in a modular structure in order to foster the implementation of additional features without rethinking the core functionality of the software, both from a technical and a user focused standpoint.

4.3.1_ General – Applied to every platform

As anticipated in the previous paragraph, every platform can be moved and scaled in the environment. Doing so, scales and moves also the respective Content. Since these actions are crucial for the proper functioning of the software and they affect a large part of the program, the researchers put particular attention on this specific feature.

The user is able to select a platform by Hovering and then Pinching. Afterwards, the user can either move the platform by pinching and holding or, enter Scale&Rotation mode. To enter this mode, the user has to use both hands. On the 3D UI, the user can check whether the software detects each hand. When both hands are detected, the user can Pinch&Hold and then move to perform the actions. Once more, the 3D UI gives a feedback on the Pinch&Hold detection. If the hands move across the X axis, the platform and its content are scaled. On the contrary, if the hands move across the Z axis, in depth, the platform and its content are rotated. Every movement on the Y axis is ignored.

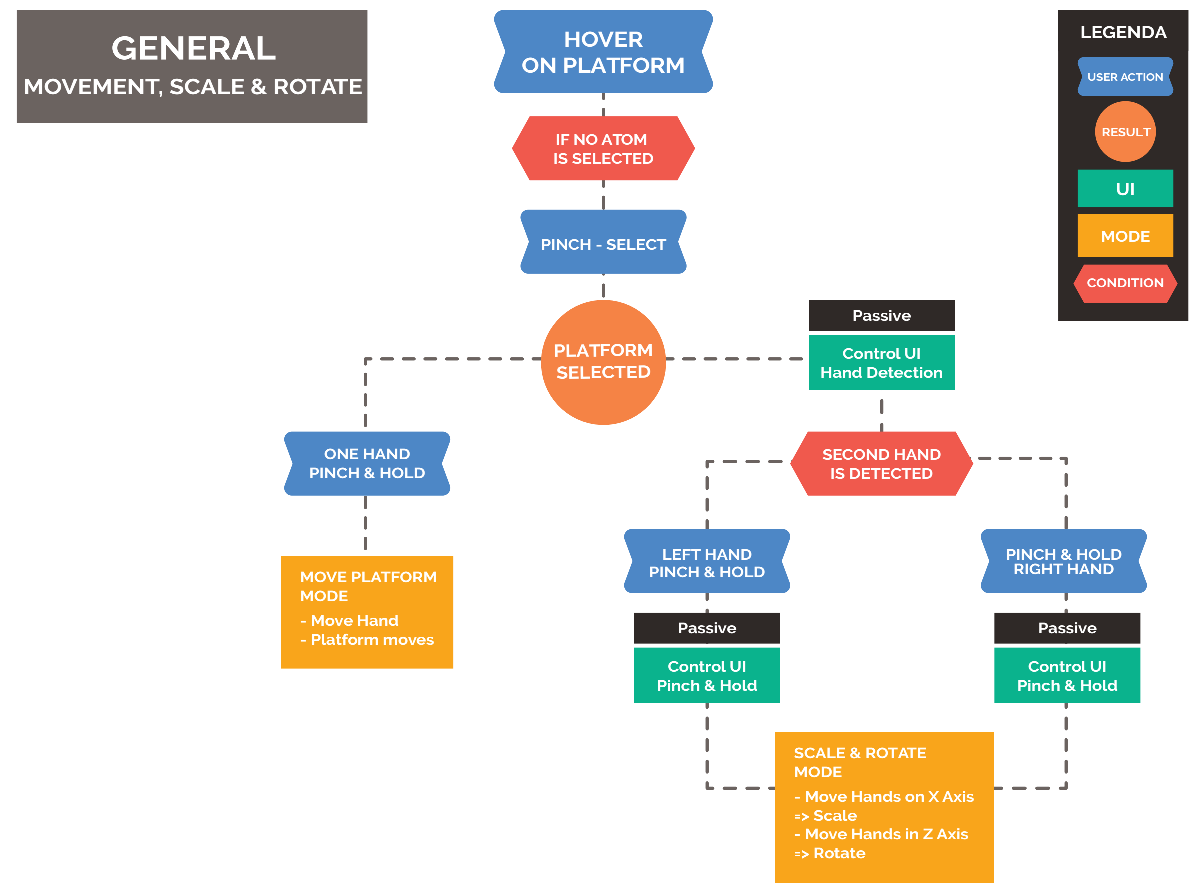


Figure 4.3 - Movement, Scale and Rotate sequence applied to all platforms

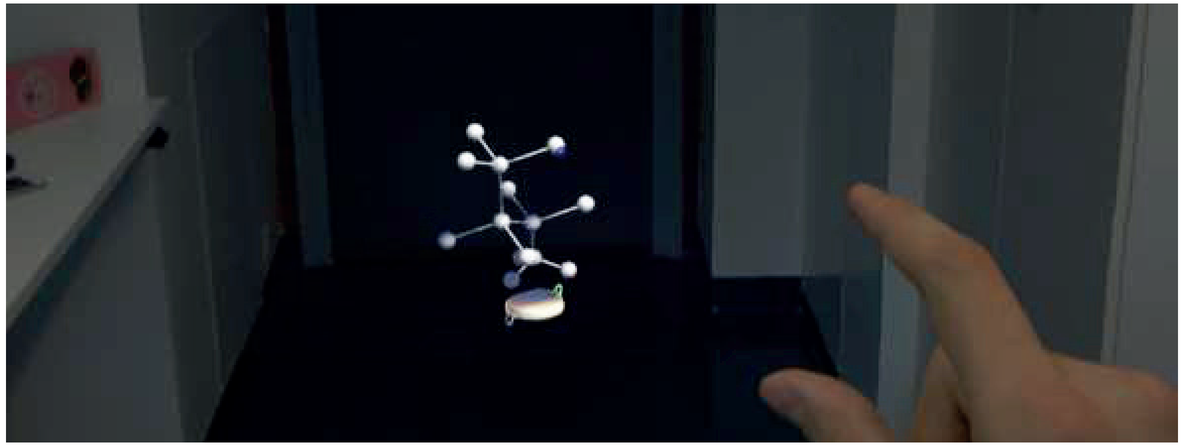


Figure 4.4 - The user pinches to select the platform

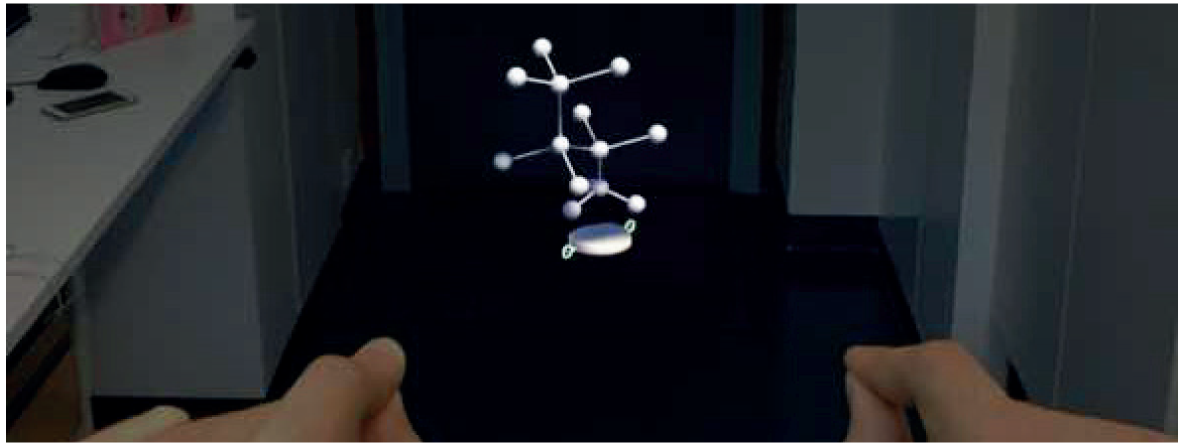


Figure 4.5 - The user pinches with both hands, adjusting the movement horizontally to scale and rotate

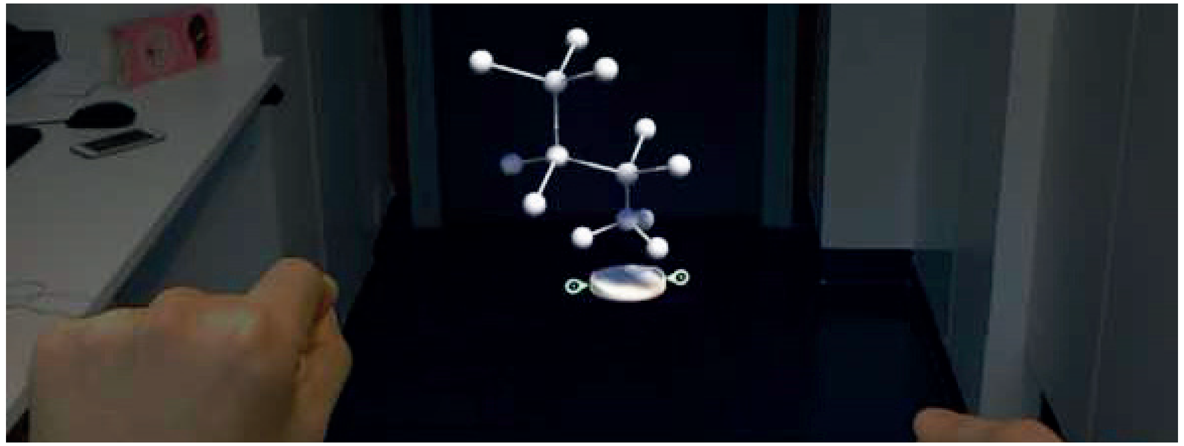


Figure 4.6 - The user moves the hand in depth to rotate the structure

4.3.2_ Main – Molecule Creation

The Main platform collects the core functionality of the software. Here the user can create, manipulate and visualize 3D molecules in the augmented space. This is the most complex platform and contains several sub menus that allow precise manipulation of specific parts of the molecules.

The Main platform's behavior is divided in two macro areas: when the user hovers on an atom, and when the hover is on an empty space. The following diagrams, part 01 and part 02, show the user flows. When the user is hovering on an atom, this can be selected. After having an active selection, the pinch and hold function, performed on the same atom, activates Create Mode. In this mode, as the user moves the hand, a new atom is created and positioned using the HoloLens' hands tracking.

The atom or the fragment instantiated is selected through the Tools platform, explained in the following sub-chapter. As soon as the Pinch and Hold is released, the atom creation is complete.

On the other hand, if the Pinch and Hold action is performed on a bond, a wheel menu opens. This menu is contextual and shows the Move and Rotation Mode. The two modes are performed exploiting the HoloLens' hand tracking as the Creation mode, allowing a precise movement, especially when using the HoloLens clicker, a small controller that detects movement and clicks.

The second part of the interaction happen when the user is hovering on an empty space with the cursor. Here, the software must check whether a selection is active or not. If a selection is active, a pinch will deselect everything, while a pinch and hold will open a wheel menu that allows to show some metric UI, such as Distance and Centre, or save the fragment into the Tool platform.

In addition, this menu offers the possibility to delete the selected atoms. This option is reachable through a wheel menu because it is important to be sure that the user is doing it willingly.

In the case the user does not have an active selection, the contextual wheel menu will show the possibility to create a new main platform, to use in parallel, or to activate Delete Mode. In this mode, the user will be able to pinch and instantly delete atoms and bonds.

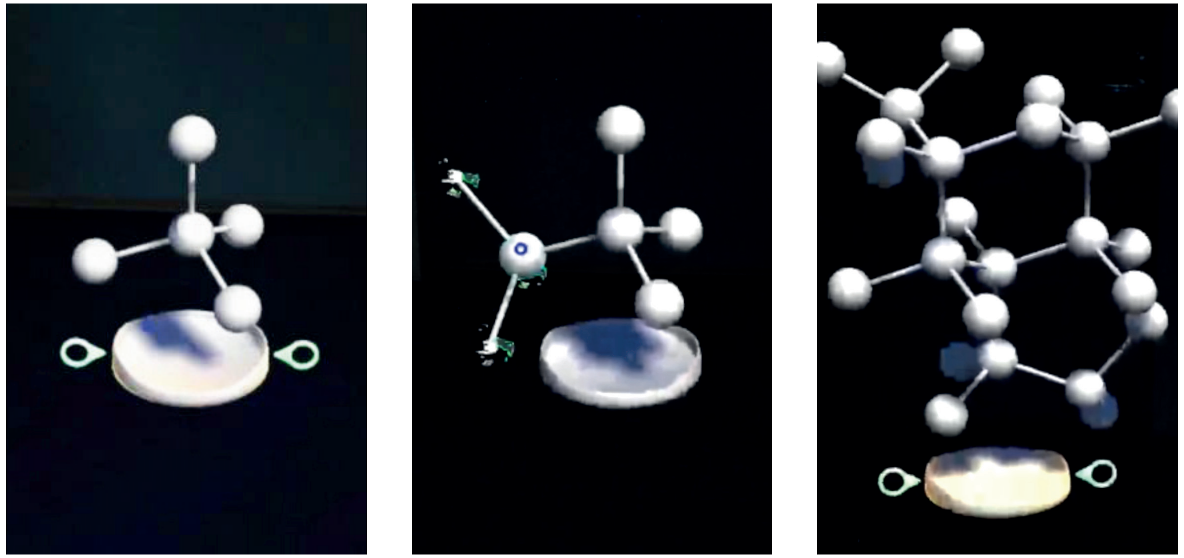


Figure 4.7, 4.8, 4.9 - Molecule creation sequence

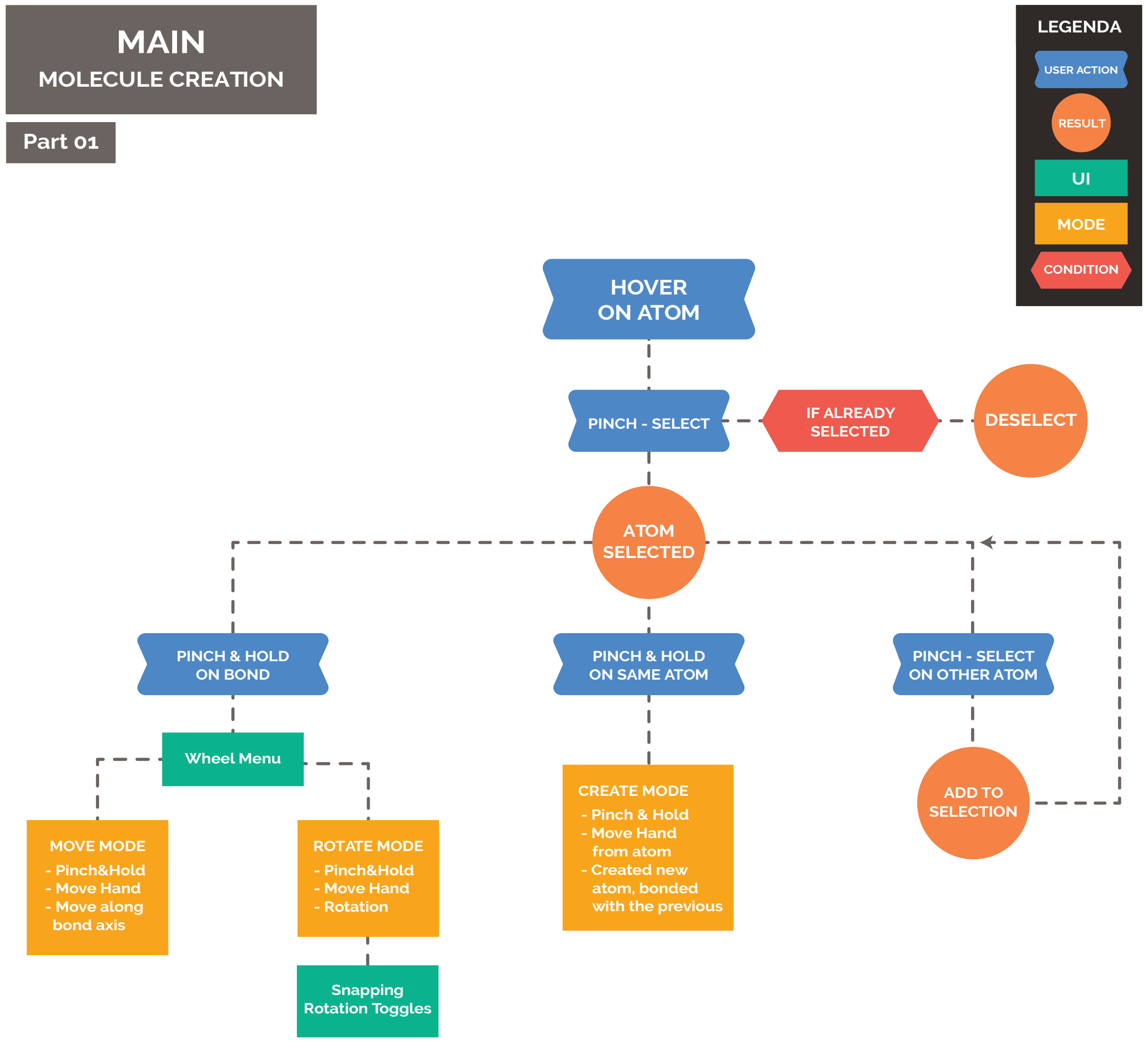


Figure 4.10 - Molecule creation, the key function of the Main platform (part 01)

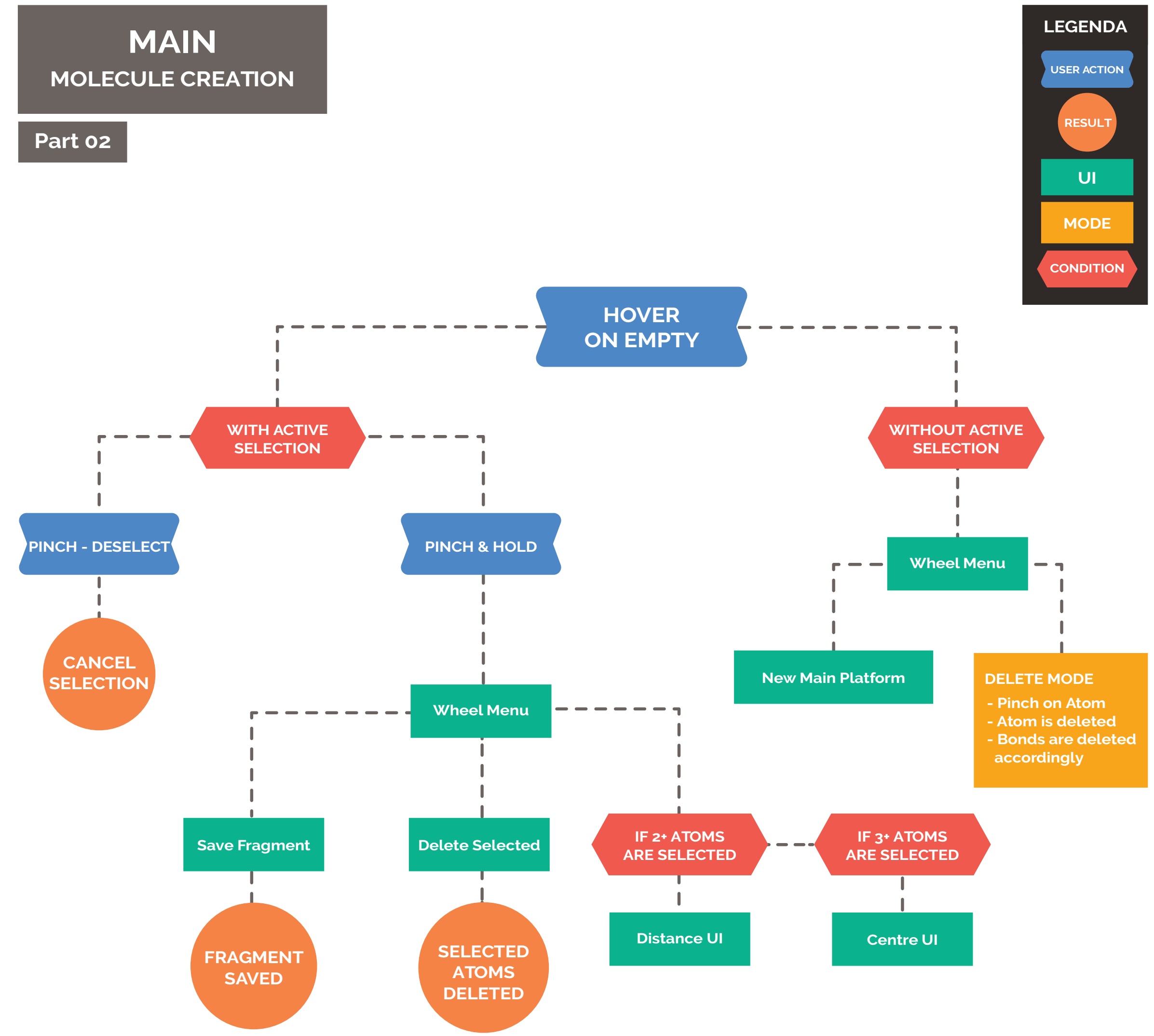


Figure 4.11 - Molecule creation, the key function of the Main platform (part 02)

4.3.3_ Tool - Atom & Fragments

The Tool platform allows the user to mark the atom or the fragment to instantiate in Create Mode. When these elements are marked as active, the user can instantiate them in the Main platform. Having both atoms and fragments is crucial for a quick use of the software. Leaving aside the complex official definition, a fragment can be defined as a sequence of linked atoms; sequences like this are extremely helpful to speed the chemists' workflow, especially when focusing on a very narrow research topic that deals with few recurring atoms types or structures to be visualized. The user can change and save custom fragments or quick access atoms, to improve the workflow speed, as most of the projects require a small variety of different atom sets.

If the user hovers on the platform and performs a Pinch and Hold action, a wheel menu appears. This menu allows to open two sections: one for atoms and one for fragments. The one for atoms is divided between common atoms and the whole periodic table. The first sub-menu is used to access quickly the atoms the user is working on, and the list can be edited by adding specific elements form the periodic table sub-menu. Regarding the fragments, the menus are similar. However, the periodic table menu is substituted by the list of custom fragments the user saved previously. Once more, all the deletion actions, both on atoms and fragments, require an additional step to ensure the willingness of the user.

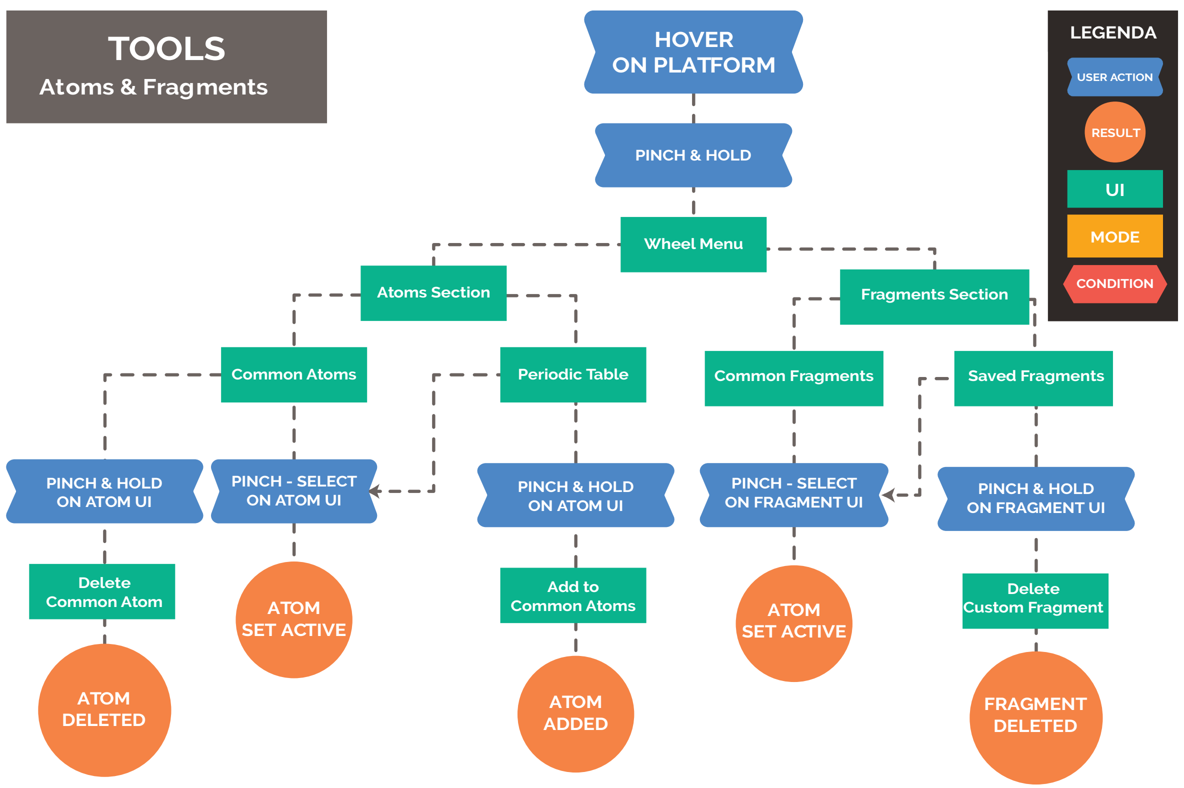


Figure 4.12 - The tools platform sequence, between atoms menu and fragments menus

4.3.4_ Utility - Undo, Redo, Geometry Optimizer

The Utility platform allows the user to perform quick actions. Upon this platform, three 3D models are present. Each model serves a function: undo the action, redo the action or toggle the geometry optimizer (G.O.).

The geometry optimizer is a function already present in the previous version of the prototype, which ensures a realistic behavior of the atoms forming the molecule, checking distance and positioning in space.

The functions linked with the Utility platform are very simple features and frequently used; for this reason, they need to be accessible at any time, without mixing with other more complex functionalities. The Utility platform should host only one-click interactions.

The user can hover on 3 different 3D Icons and perform the corresponding actions just by pinch-select on them. This ensures a quick workflow and, as a concept, it's the equivalent of a CTRL+Z shortcut on a keyboard.

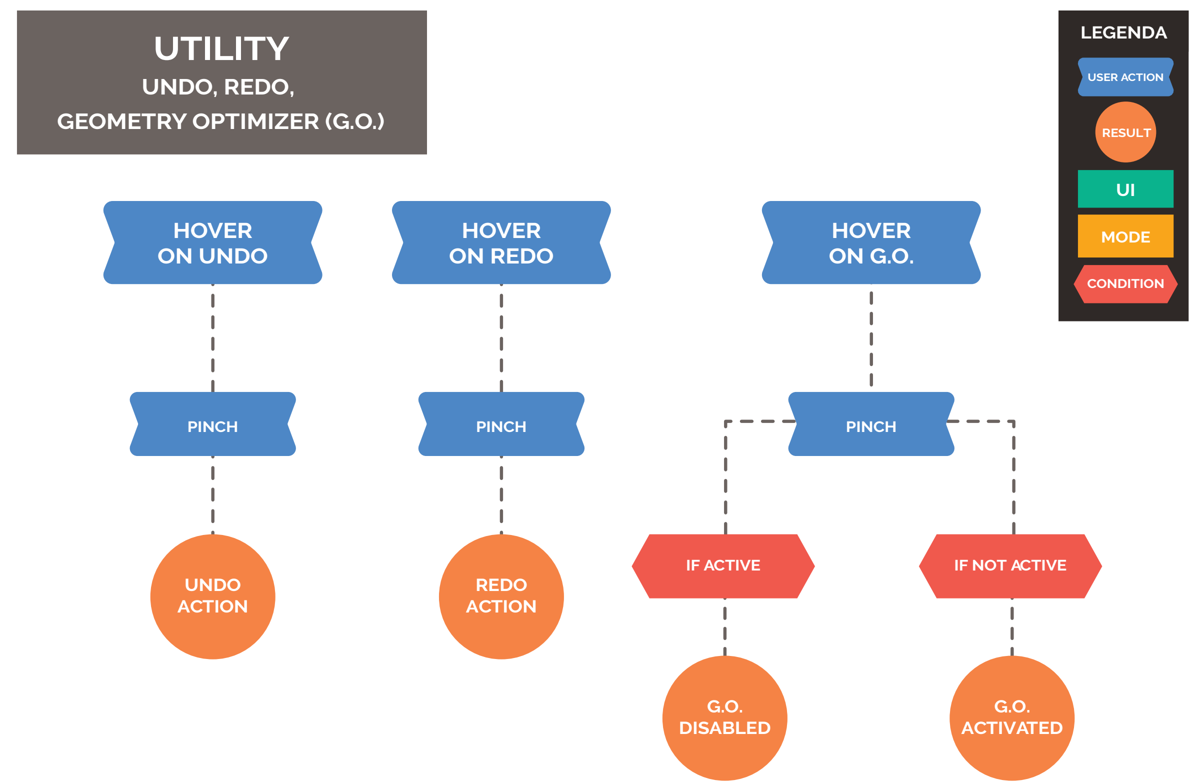


Figure 4.13 - The utility platform has simple flows focused on quick one-pinch interactions

4.3.5_ System - Save, Load & Delete

The System platform is dedicated to every need that in a desktop PC program could be found in the "file" tab. For the prototype, only a small set of system function was considered: the possibility to save and load project files, a function to delete the current project and one last to import molecules from other software.

Loading files, especially from other programs, was considered crucial. This comes from the need for visualization, one of the key findings emerged from the background research. Additionally, if the user pinches on the platform, a quick save is performed. This allows a smooth workflow without interruptions, just as in normal desktop software.

In the System platform, the user can mainly manage files through the HoloLens' built-in system interface. Considered the scope of the prototype, as well as the quality of the existing menus, designing new ones felt unnecessary.

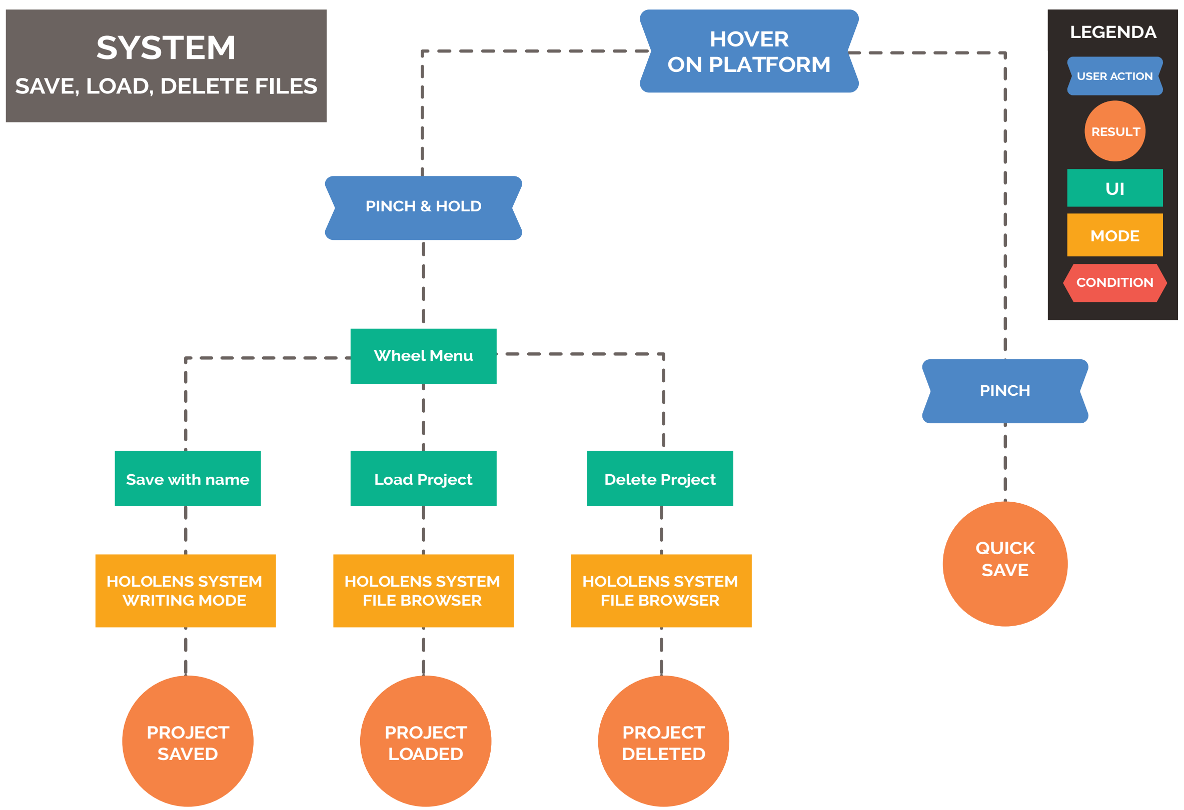


Figure 4.13 - The System platform is the most simple one as it focuses on Windows built-in operations

4.4_ Action Sequences

For implementation purposes, several sequences of user flows were created. These paths are detailed steps to be followed and tested during the implementation, aiming to give all the information needed to the user on one side, and granting clarity and smoothness on the programming side.

Some parts might overlap with the previously explored flows, however, here the focus is on the detailed step by step implementation. The following lists could be difficult to follow if not familiar with the project, however they are meant to be used as guidance by developers in future expansions of the project.

1. Introduction Sequence

1 . Title UI Screen
2 . UI Message: "mapping the surroundings"
3 . Visual shader highlights the map
4 . UI Message: "Mapping completed"
5 . Proceed button, to be pressed
6 . First Platform Sequence

2. First Platform Sequence

1. A platform is created automatically on the gaze position
2. The platform follows the gaze with a smooth delay
3. UI Message linked to the object: "place the platform by clicking"
4. When clicking, the platform is placed
5. UI text disappears

3. Atom Label UI Sequence

1. If the cursor stays more than 2 seconds on an atom
2. A label with the atom symbol appears

4. Atom Selection Sequence

1. The Atom is selected
2. The Atom is highlighted
3. The bonds are soft-lighted

5. 3D UI Platform Selection Sequence

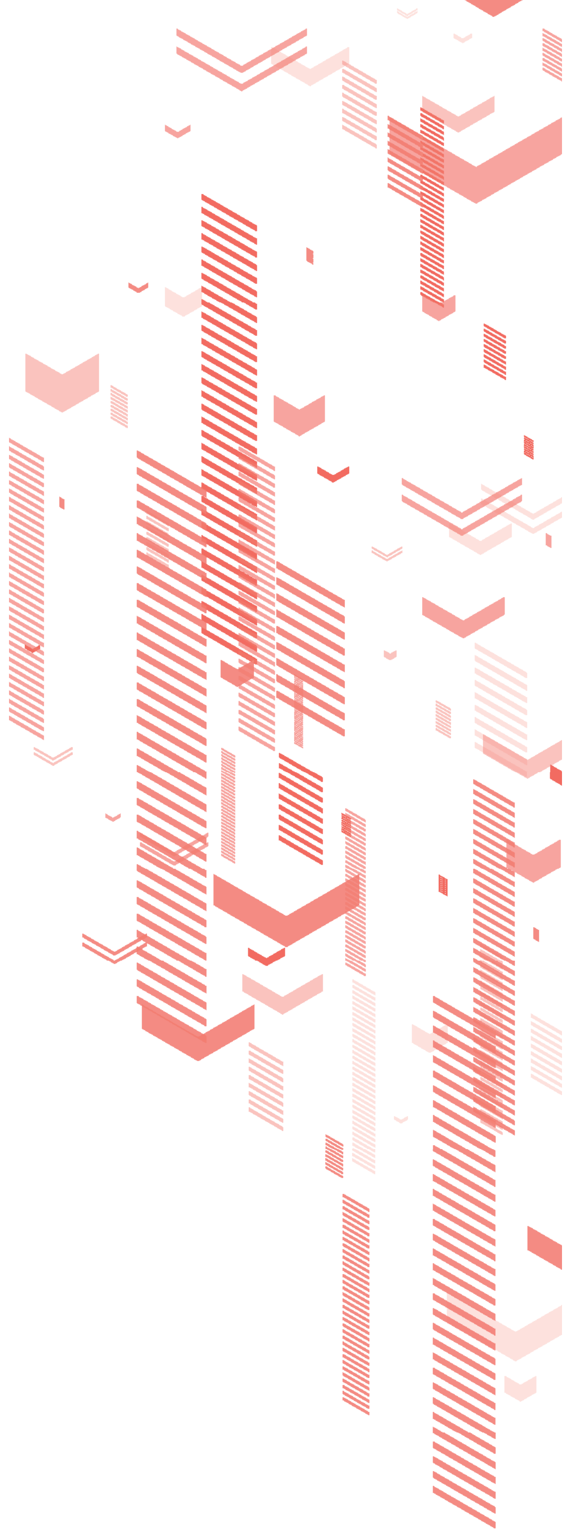
1. Soft Highlight on cursor over
   1.5) Scale/Rotate/Move 3D UI appears with a semi-transparent shader
2. Click to select
3. Highlight when selected
   3.5) Scale/Rotate/Move are now rendered opaque
4. Move 3D UI appears in the center of the model
5. Scale/Rotate 3D UI appears on the sides

6. 3D UI Platform Scale/Rotation Sequence

1. Handles highlight when the respective hand is recognized
2. Handles change shape when pinch&hold
3. Handles change colour when the Rotation/Scale is activated
4. The colour is relative to the scale/rotation parameters
5. Handles follow the movement of the hands in space
6. The hands set the rotation factor, but the action is continuous
7. Handles are locked on the X axis

7. 3D UI Platform Movement Sequence

1. Pinch&Hold activates movement mode - One hand detected
2. Move 3D Icon appears while Pinch&Hold
3. Highlights and changes colour when moving
4. The icon rotation is affected by movement
   (e.g. if the platform moves towards the user, the icon leans in the same direction)

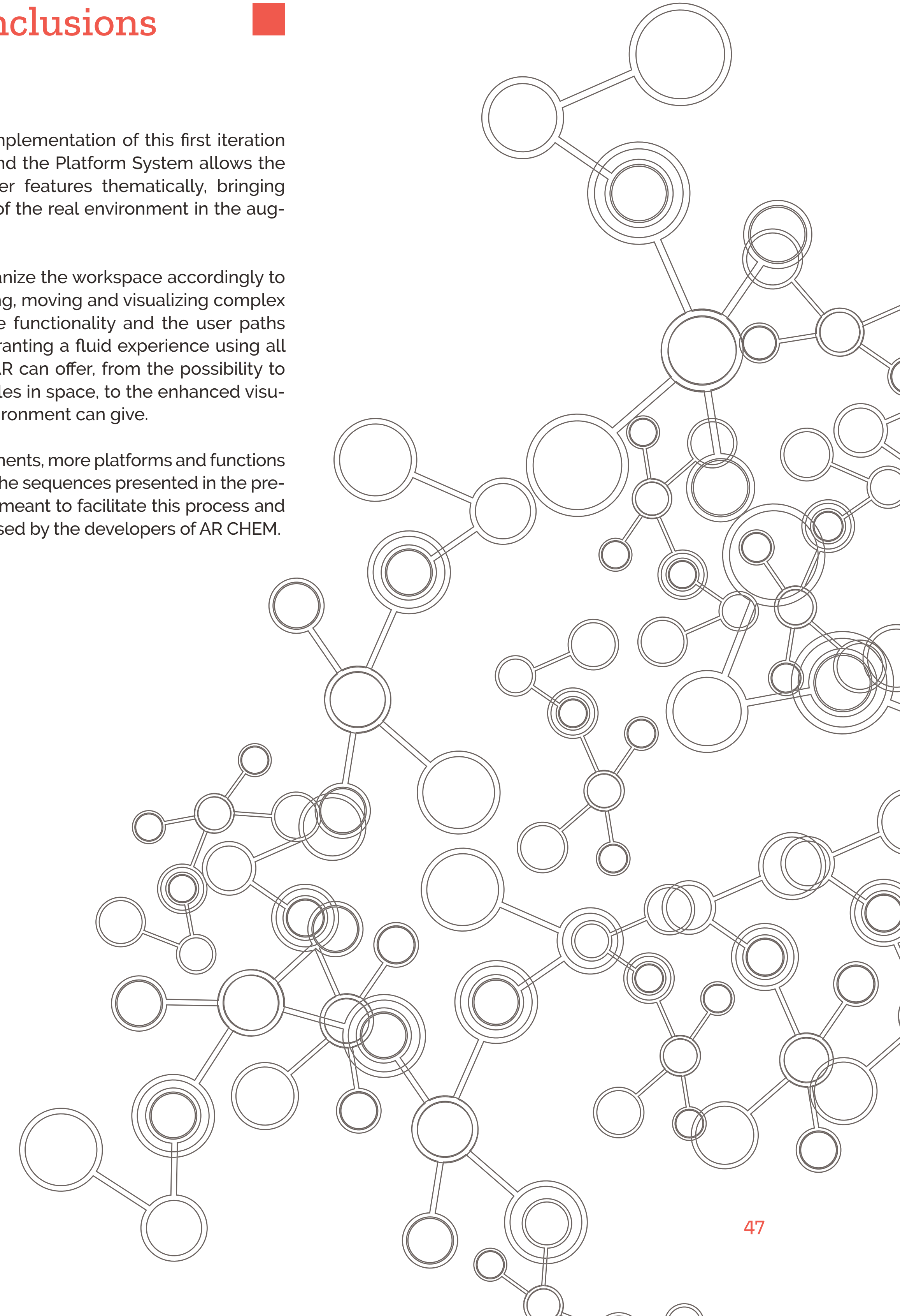


4.5_ Conclusions

The suggested implementation of this first iteration of the 3D Icons and the Platform System allows the software to gather features thematically, bringing the intuitiveness of the real environment in the augmented world.

The user can organize the workspace accordingly to their needs, scaling, moving and visualizing complex molecules. All the functionality and the user paths are focused on granting a fluid experience using all the feature that AR can offer, from the possibility to collocate molecules in space, to the enhanced visualization a 3D environment can give.

In future developments, more platforms and functions could be added. The sequences presented in the previous chapter are meant to facilitate this process and are meant to be used by the developers of AR CHEM.



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Appendix (A) - HoloLens Technical Specifications

This appendix presents the complete feature list of HoloLens, retrieved from:
https://docs.microsoft.com/en-us/windows/mixed-reality/hololens-hardware-details

01. Optics

- See-through holographic lenses (waveguides)
- 2 HD 16:9 light engines
- Automatic pupillary distance calibration
- Holographic Resolution: 2.3M total light points
- Holographic Density: > 2.5k radiants (light points per radian)

02. Sensors

- 1 IMU
- 4 environment understanding cameras
- 1 depth camera
- 1 2MP photo / HD video camera
- Mixed reality capture
- 4 microphones
- 1 ambient light sensor

HoloLens optics and tracking system, retrieved from https://docs.microsoft.com/

03. Human Understanding

- Spatial sound
- Gaze tracking
- Gesture input
- Voice support

04. Input / Output / Connectivity

- Built-in speakers
- Audio 3.5mm jack
- Volume up/down
- Brightness up/down
- Power button
- Battery status LEDs
- Wi-Fi 802.11ac
- Micro USB 2.0
- Bluetooth 4.1 LE

05. Power

- Battery Life
- 2-3 hours of active use
- Up to 2 weeks of standby time
- Fully functional when charging
- Passively cooled (no fans)

06. Processors

- Intel 32 bit architecture with TPM 2.0 support

07. Weight

- 579g

08. Memory

- 64GB Flash
- 2GB RAM

HoloLens motherboard, retrieved from https://docs.microsoft.com/

09. OS and Apps

- Windows 10
- Windows Store
- Holograms
- Microsoft Edge
- Photos
- Settings
- Windows Feedback
- Calibration
- Learn Gestures
- Custom-built Microsoft Holographic Processing Unit (HPU 1.0)

10. What's in the box

- HoloLens Development Edition
- Clicker
- Carrying case
- Charger and cable
- Microfiber cloth
- Nose pads
- Overhead strap

Appendix (B) - Focus group agenda and interview questions

Focus Group Agenda

5 participant x 45 minutes

- Project introduction
- Questions and discussion
- AR CHEM explanation
- Questions and discussion

Aim: scoping AR Chem

- Identifying the purpose of AR Chem
- Confirming where Augmented Reality is adding value for the user
- Confirming the basic key feature set
- Identifying possible features to improve the current software
- Identifying UX pitfalls
    - *Understanding current software workflows*
    - *Identifying conventions and known methodologies*

Profiling:

Title/ Specialization	*Years of Experience*	*Programs utilized*	*Frequency of use*	*Main reason for use*

Profiling form: https://francescofontana.typeform.com/to/YQ1cFo

Focus group questions:

01. How are molecular visualization software part of your workflow?

02. Are you satisfied with the programs?

03. Could you describe the basic features?

04. What's the most useful feature?

05. What are the flaws?

06. How could they be tackled?

Overview and presentation of AR CHEM feature set

07. Do you agree with the feature set?

08. What other features would you add?

EXTRA

09. Can you think about an example of collaboration during molecular manipulation?

10. Can you see yourself working with HoloLens in the future?

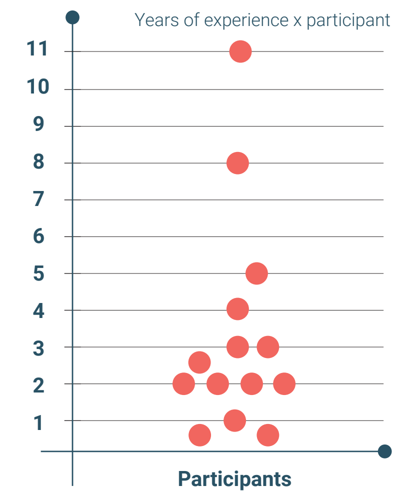
Appendix (C) - Focus group results

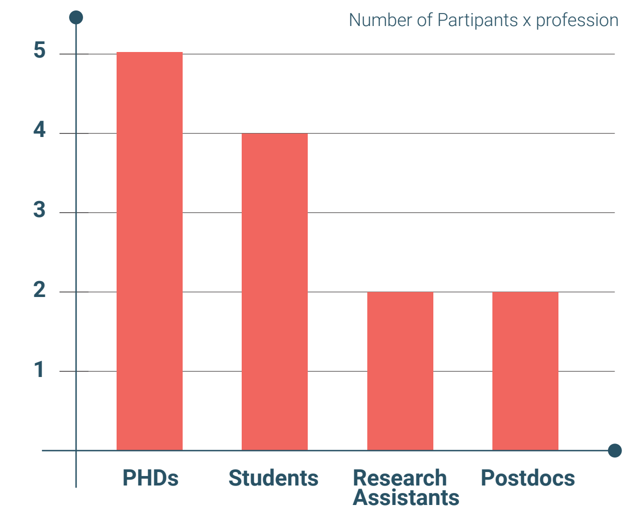
14 Participants

6 Expert Users

60+ Insights

3 Workshops





Chemists needs and wants

- Tweak structures
- Build
- Visualize
- Find Symmetries
- Insert atom groups
- A Jack of All Trades program
- Experiment with parameters
- Use Text files between programs
- Mirroring
- Step by step feedback on an animation
- Structure beakdown for education
- Understanding chemical reactions in 3D

Softwares and best features

JMOL
- Easy substitution of Atoms
- Input/Output file management
- Simple User Interface
- Change color of objects
- Imbedding into websites
- Interpreting files from a simulation

MATERIAL STUDIO
- Easy manipulation
- Big set of different features

VESTA
- Pretty visualizations
- Ballsticks/Polyhedron quick shift
- Easy to use
- Lightweight and fast

CRISTAL MAKER
- Allows asymmetrical manipulation
- Calculates the ideal centre
- Calculates the vector between an atom and a centre

MERCURY
- Easy to switch between structures
- Good list of structures available

PV
- Different visualization styles
- Structure comparison

CHEMCRAFT
- Good atoms manipulation
- Easy to use

Common programs flaws

- No actions history
- Outdated UI
- No customizable settings
- Unclear language
- The programs don't have a standard exchange format to share files
- Can't move a specific part of the structure
- Can't compare structure
- The visualization is clear but looks bad

AR CHEM - Feedback & Missing Features

- Render option
- View Modes
- Align Groups
- Add Notes
- Visualize free electron pairs
- Visualize polyhedral structure
- List of common groups
- Display atoms names
- Mirroring
- Save&Add unique fragments
- Animations
- Using bonds as attachment point for fragments
- Import Structures
- Hovering
- Autosave